Supporting Information for

Reactions of Group III Biheterocyclic Complexes

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Experimental

Synthesis of $LuCl_3$. $LuCl_3$ was prepared in the same manner as reported for $ScCl_3$.[1]

Lu_2O_3 (10 g, 0.025 mol) and NH_4Cl (40.3244 g, 0.754 mol) were combined in a 1 L Erlenmeyer flask and dissolved in 500 mL H_2O : concentrated HCl (1:1 ratio by volume). This solution was stirred with gentle warming overnight, while a slight flow of air was directed over the flask. The still damp white solid was then ground up with a mortar and pestle. The solid was placed in a Pyrex vacuum trap (approximate dimensions: 5 cm diameter, 30 cm length) equipped with a number 40 o-ring glass joint. A Pyrex tube equipped with a male number 40 glass joint (approximate length, 15 cm) and a stopcock at the opposite end was fitted to the vacuum trap. The vacuum trap up to the joint was placed in a tube furnace (the joint itself should not be placed in the furnace). The apparatus was then heated under dynamic vacuum to 413 K, 523 K, and 633 K, for 24 h each. The apparatus was removed from the furnace, cooled, and brought directly into the glove box. Yield 12.1975 g of a gray powder, 86%.

Synthesis of $Lu(CH_2Xy\text{-}3,5)_3(THF)_2$. $LuCl_3$ (1.022 g, 3.633 mmol) was measured into a 100 mL round bottom flask with about 50 mL of a 2:1 mixture of THF : hexanes by volume, and then frozen at -196 °C. $K(CH_2Xy\text{-}3,5)$ (1.500 g, 9.477 mmol) was measured into a 20 mL vial and then cooled to -196 °C. These first steps were then repeated so that two reactions could be done in parallel and combined later, for a total of 2.044 g $LuCl_3$ (7.266 mmol) and 3.000 g $K(CH_2Xy\text{-}3,5)$ (18.95 mmol). After cooling, approximately half of the $K(CH_2Xy\text{-}3,5)$ (~0.75 g for each reaction being done) was added to each of the round bottom flasks. The solutions were then stirred at 0° C for 30 min, after which the remaining $K(CH_2Xy\text{-}3,5)$ was added to each reaction. The solutions were then allowed to stir for 2.5 h at 0° C. At this point, all reactions being done in parallel were combined and filtered through Celite. The solution was next dried under vacuum, resulting in an orange powder. The solid was taken up in a 1:1 ratio by volume of toluene : hexanes in order to precipitate any salts (extra hexanes may be added as necessary to help precipitate salts). The solution was filtered through Celite and dried, leaving a yellow powder, which should be readily soluble in toluene. If the product is only slightly soluble in toluene, it may be indicatory of the formation of $[Lu(CH_2Xy\text{-}3,5)_4(THF)_x]^-$, "-ate" salt, which has been previously observed in our lab for the Lu complex, as well as for corresponding Y and Sc complexes.[1] The solid was then crystallized from toluene layered with pentane, giving $Lu(CH_2Xy\text{-}3,5)_3(THF)_2$ as white feathery crystals. Yield 1.8366 g, 43%.

Note: The product, $Lu(CH_2Xy\text{-}3,5)_3(THF)_2$, is best used immediately because it starts to decompose after ~2 weeks when stored at -35 °C.

^{1}H NMR (500 MHz, C_6D_6): δ, ppm: 6.46 (s, 6H, aryl-C*H*), 6.44 (s, 3H, aryl-C*H*), 3.52 (br, 8H, OC*H*$_2$CH$_2$), 2.27 (s, 18H, C*H*$_3$), 1.60 (s, 6H, benzyl-C*H*$_2$), 1.16 (br, 8H, OCH$_2$C*H*$_2$). ^{13}C NMR (126 MHz, C_6D_6): δ, ppm: 151.9, 137.8, 122.4, 120.3, 71.2, 58.3, 25.2, 21.9.

Anal. for $C_{35}H_{49}O_2Lu$: Calcd.: C, 62.12%; H, 7.30%; N, 0.00%. Found: C, 61.78%, H, 7.20%, N, ND<0.20%.

Synthesis of $Lu(fc[NSi^tBuMe_2]_2)(CH_2Xy\text{-}3,5)(THF)$, $\mathbf{1^{Lu}}$-THF

Note: The procedures listed below describe a typical synthesis of **1^{Lu}-THF** in our lab. Several reactions are run in parallel. These reactions are then combined at the filtration step. However, so far no loss in % yield has been observed when the reaction is run on a larger scale. Thus, it may not be necessary to run several reactions in parallel.

In a typical synthesis, four reactions were run in parallel. $Lu(CH_2Xy\text{-}3,5)_3(THF)_2$ (1.6410 g, 2.4250 mmol) was carefully measured into 4 vials to give approximately 410.3 mg per vial. The ligand $fc[NHSi^tBuMe_2]_2$ (1.0781 g, 2.4250 mmol) was carefully measured into 4 vials to give approximately 269.5 mg per vial. At this point, the solids $fc[NHSi^tBuMe_2]_2$ and $Lu(CH_2Xy\text{-}3,5)_3(THF)_2$ were each dissolved in 1-2 mL of toluene and frozen at -196°C. After allowing the solutions to thaw slightly, $fc[NHSi^tBuMe_2]_2$ was added to $Lu(CH_2Xy\text{-}3,5)_3(THF)_2$ in a 1 : 1 stoichiometric ratio (the parallel reactions are still kept separate at this point). The four orange solutions were stirred at room temperature for 3 h, after which ~5 mL hexanes was added to each reaction. The parallel reactions were combined and filtered through Celite. The orange solution was then dried under vacuum, giving an orange powder. The solid was taken up in hexanes. The solution was concentrated under vacuum and cooled to -35 °C overnight to yield orange crystals. The mother liquor was then decanted, concentrated under vacuum, and cooled to -35°C to yield further crops of crystals. As many as 4 crops of crystals were attained in this manner. Total yield: 1.8029 g, 92.0%.

^{1}H NMR (500 MHz, C_6D_6): δ, ppm: 6.96 (s, 2H, aryl-C*H*), 6.42 (s, 1H, aryl-C*H*), 3.95 and 3.24 (br s, 8H, fc-C*H*), 3.77 (br s, 4H, OC*H*$_2$CH$_2$), 2.28 (s, 2H, benzyl-C*H*$_2$), 2.27 (s, 6H, xylyl-C*H*$_3$), 1.31 (br, 4H, OCH$_2$C*H*$_2$), 1.02 (s, 18H, SiC(C*H*$_3$)$_3$), 0.22 (s, 12H, (Si(C*H*$_3$)$_2$)$_2$). ^{13}C NMR (126 MHz, C_6D_6): δ, ppm: 153.2, 138.4, 122.4, 120.7, 104.3, 71.5, 66.9, 66.7, 57.7, 28.0, 25.1, 22.0, 20.8, -1.7.

Anal. for $C_{35}H_{57}N_2Si_2OFeLu$. Calcd.: C, 51.97%; H, 7.10%; N, 3.46%. Found: C, 51.93%, H, 7.25%, N, 3.60%.

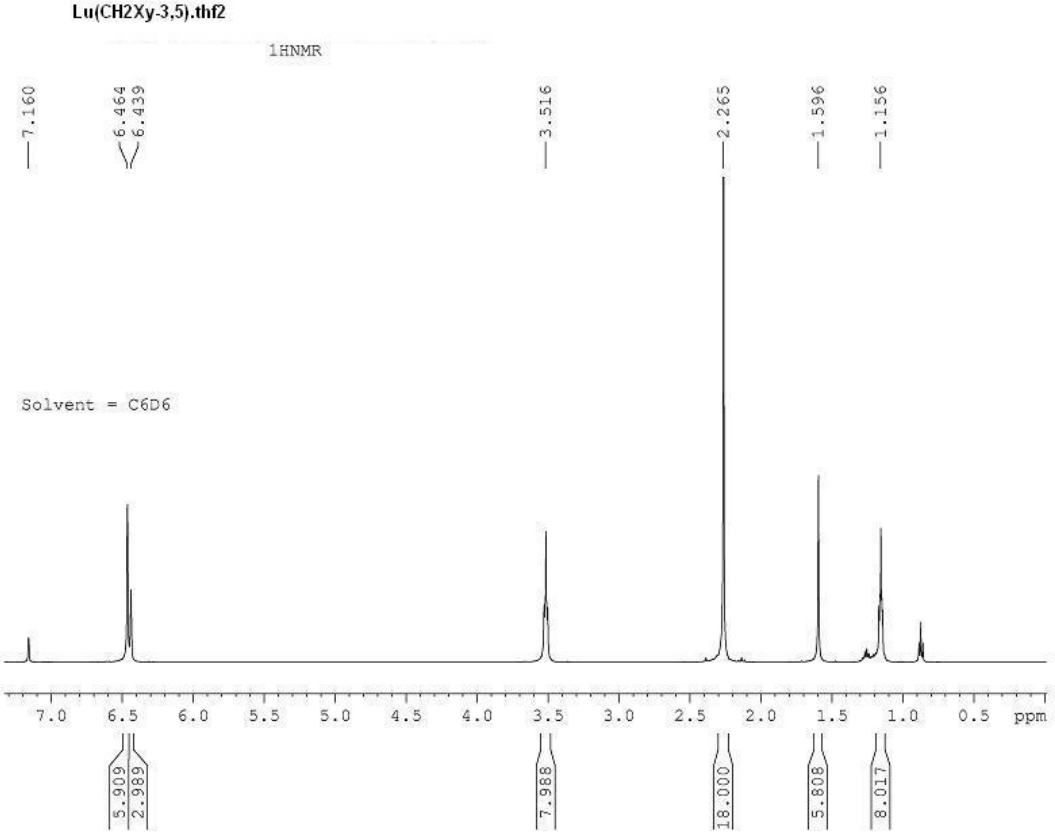
Synthesis of deuterated 3-methylisoquinoline. Deuterated 3-methylisoquinoline was prepared by a slightly modified literature procedure.[2] 3-methylisoquinoline (500 mg, 3.49 mmol) and 400 mg ruthenium on carbon (5% by wt. Ru) were placed in a 500 mL Schlenk flask along with C_6D_6 (15 mL). The flask was quickly evacuated and charged with 10 psi D_2. The reaction was allowed to stir for 4 days at room temperature. The reaction mixture was filtered through Celite and the C_6D_6 was removed. The crude product was crystallized from hexanes and used without further purification. ^{1}H and ^{2}H NMR spectroscopy showed ca. 40% deuterium incorporation at the 1 position and 33% deuterium incorporation at the 3-methyl position.

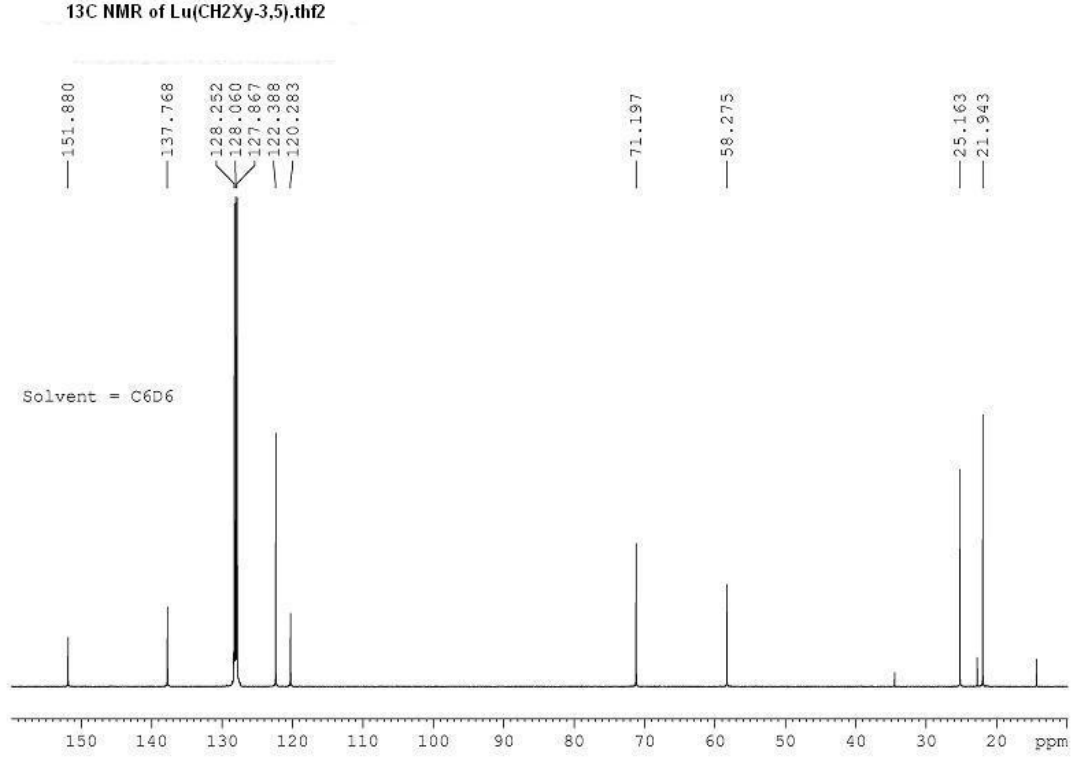
Conversion of 6^{Y}-py^{Ph}-iqn to 7^{Y}-py^{Ph}-iqn. Compound **6^{Y}-py^{Ph}-iqn** was heated at 70 °C in C_6D_6 in a J. Young tube. The transformation was monitored using ^{1}H NMR spectroscopy. Up to ~62% conversion to **7^{Y}-py^{Ph}-iqn** took place over the course of six days. Further heating resulted in no additional conversion. The ^{1}H NMR spectrum of the product closely matched that of **7^{Sc}-py^{Ph}-iqn**. However, **7^{Y}-py^{Ph}-iqn** could not be isolated.

Conversion of 6^{Lu}-py^{Ph}-iqn to 7^{Lu}-py^{Ph}-iqn. Compound **6^{Lu}-py^{Ph}-iqn** was heated at 85 °C in C_6D_6 in a J. Young tube. The transformation was monitored using ^{1}H NMR spectroscopy. Up to ~67% conversion to **7^{Lu}-py^{Ph}-iqn** took place over the course of three days. Further heating resulted in no additional conversion. The ^{1}H NMR spectrum of the product closely matched that of **7^{Sc}-py^{Ph}-iqn**. However, **7^{Lu}-py^{Ph}-iqn** could not be isolated.

NMR spectra

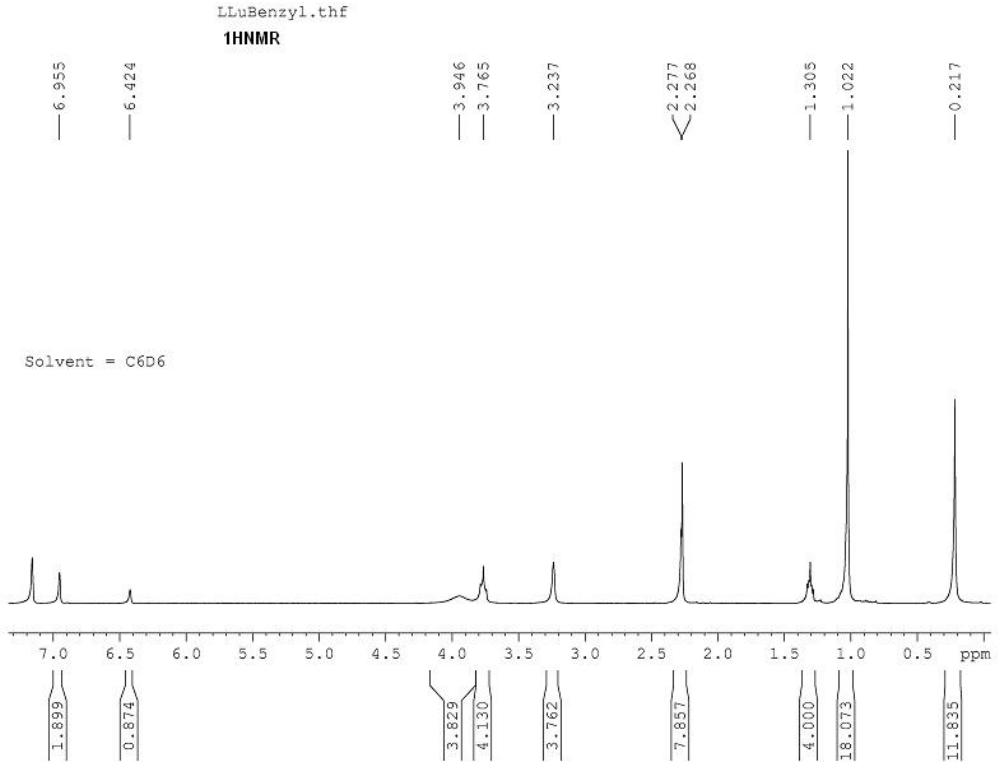
$Lu(CH_2Xy\text{-}3,5)_3(THF)_2$: Solvent peaks for pentane are also present.



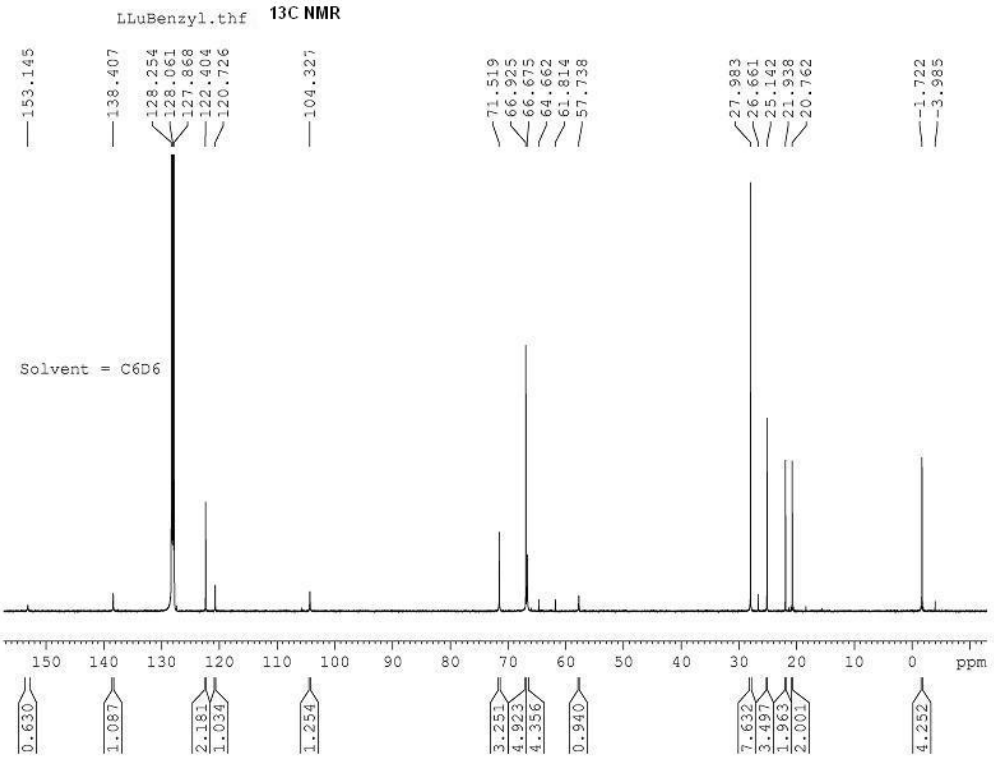


1^{Lu}-THF

^{1}H NMR (500 mHz, C_6D_6):

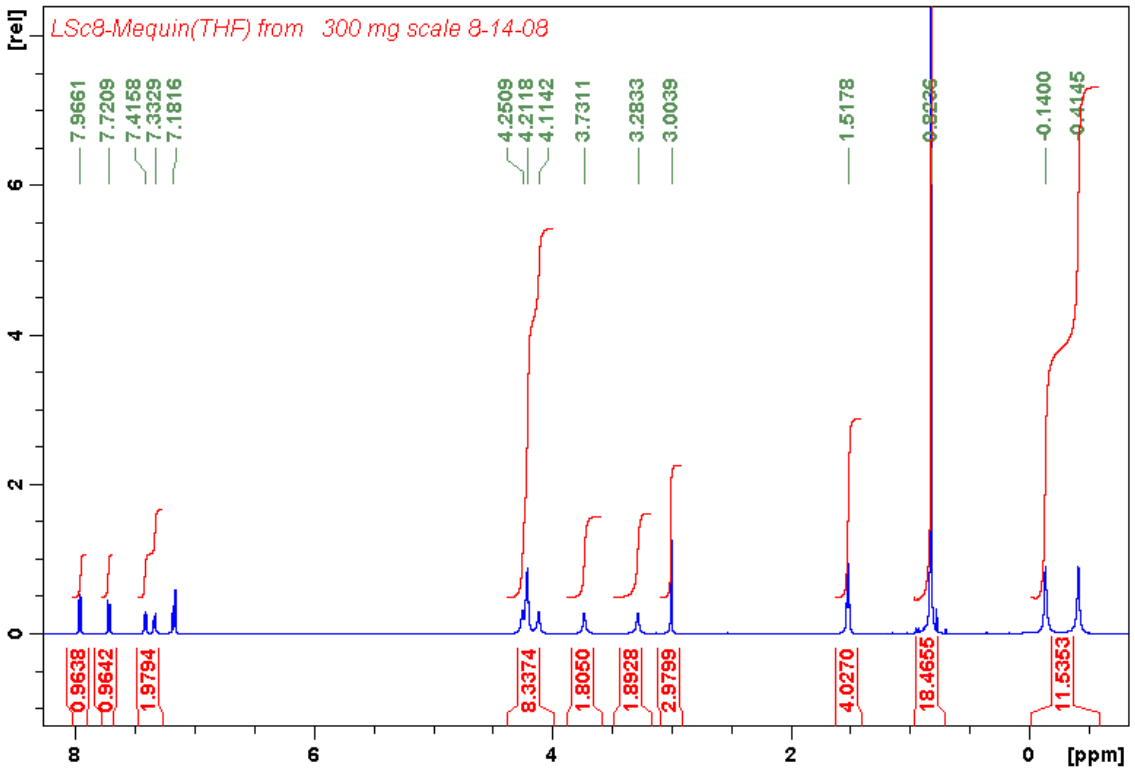


^{13}C NMR (126 mHz, C_6D_6): Peaks at 64.7, 61.8, 26.6, and -4.0 are due to a small amount of free ligand.

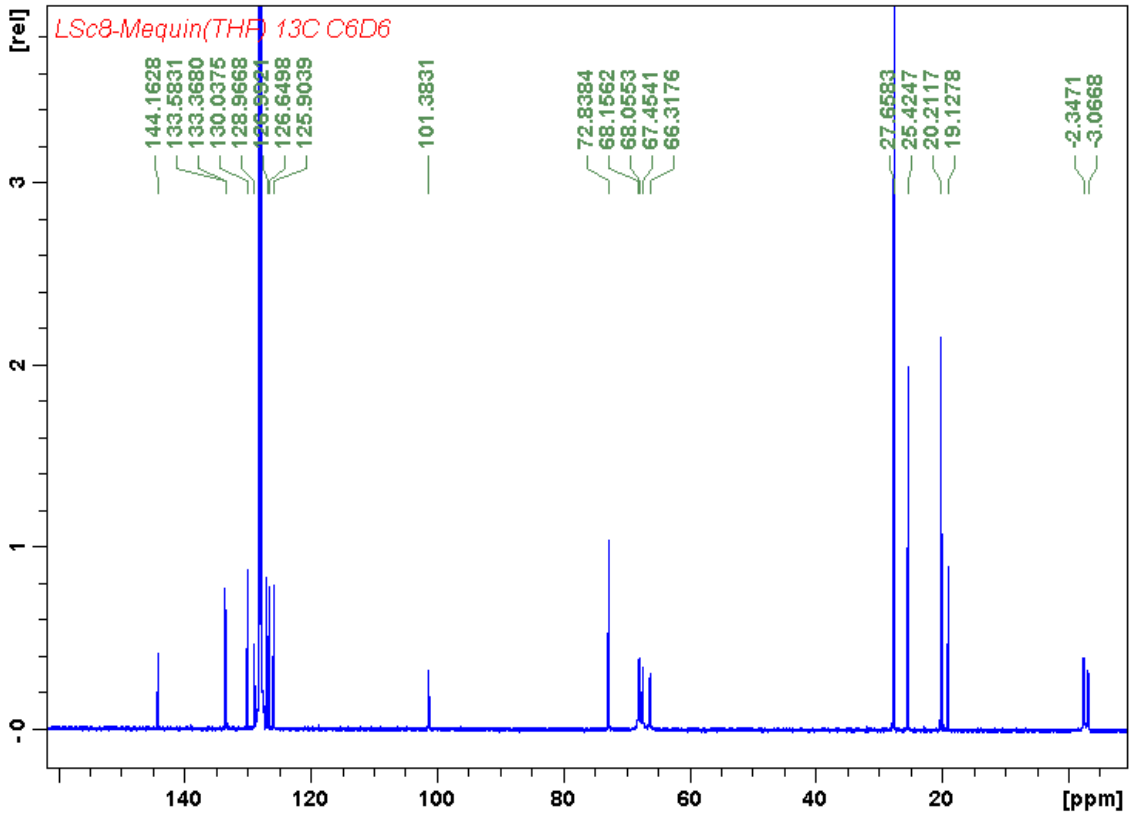


5^{Sc}-qn

^{1}H NMR (500 mHz, C_6D_6):

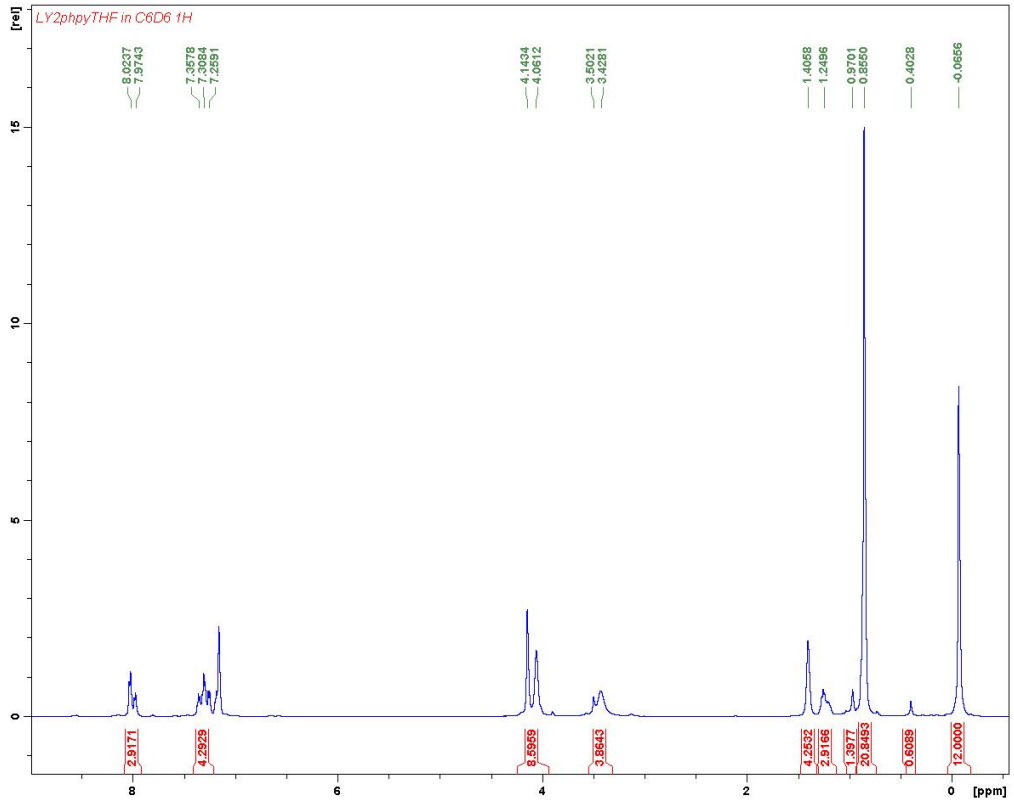


^{13}C NMR (126 mHz, C_6D_6):

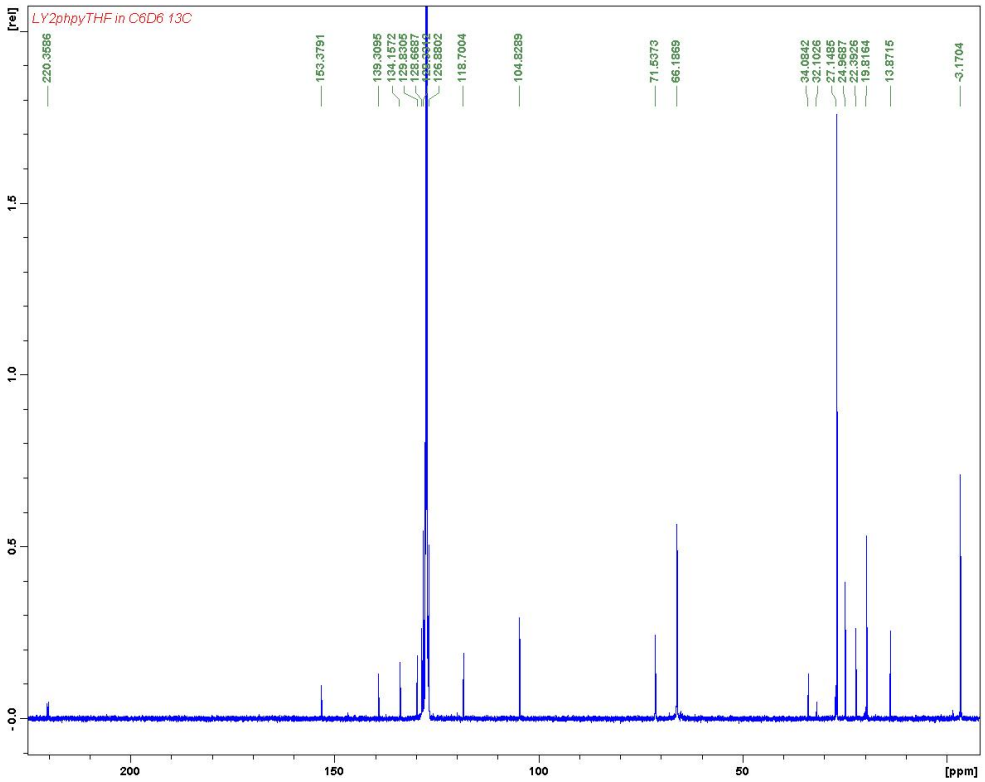


5^{Y}-py^{Ph}

^{1}H NMR (500 mHz, C_6D_6, peaks at 1.25 and 0.97 are from pentane and free THF):

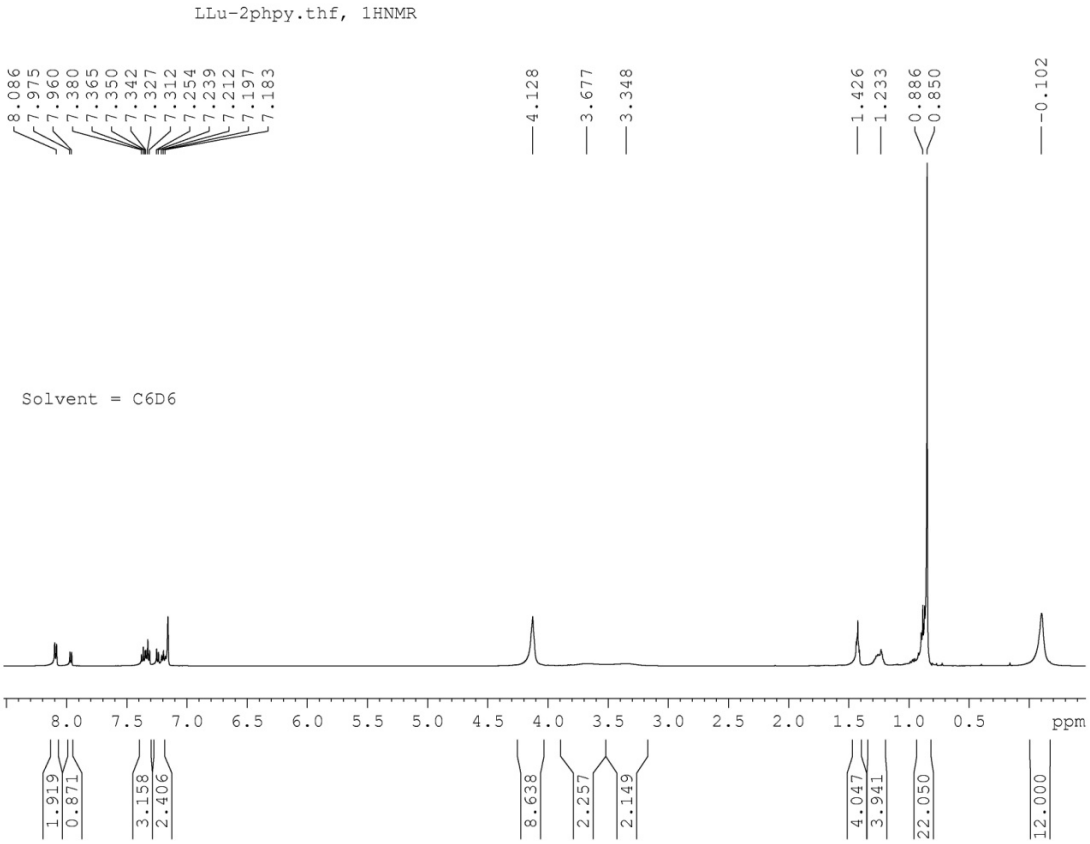


^{13}C NMR (126 mHz, C_6D_6):

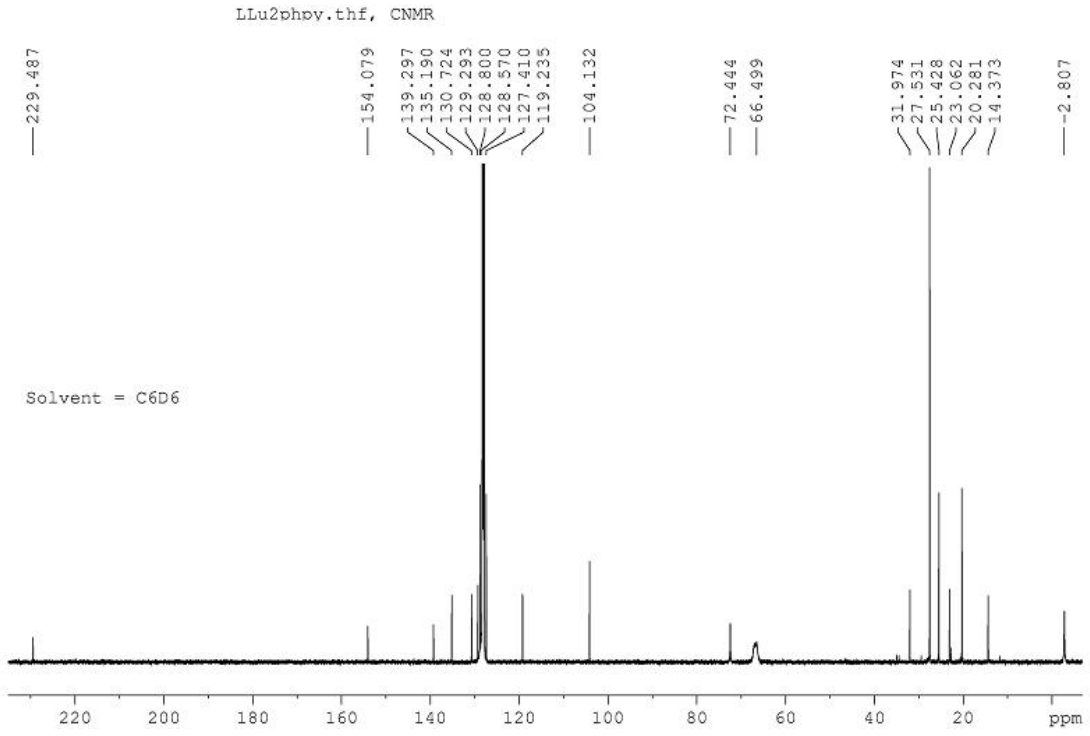


5^{Lu}-py^{Ph}

^{1}H NMR (500 mHz, C_6D_6). Solvent peaks for hexanes are present at 1.23 and 0.89.

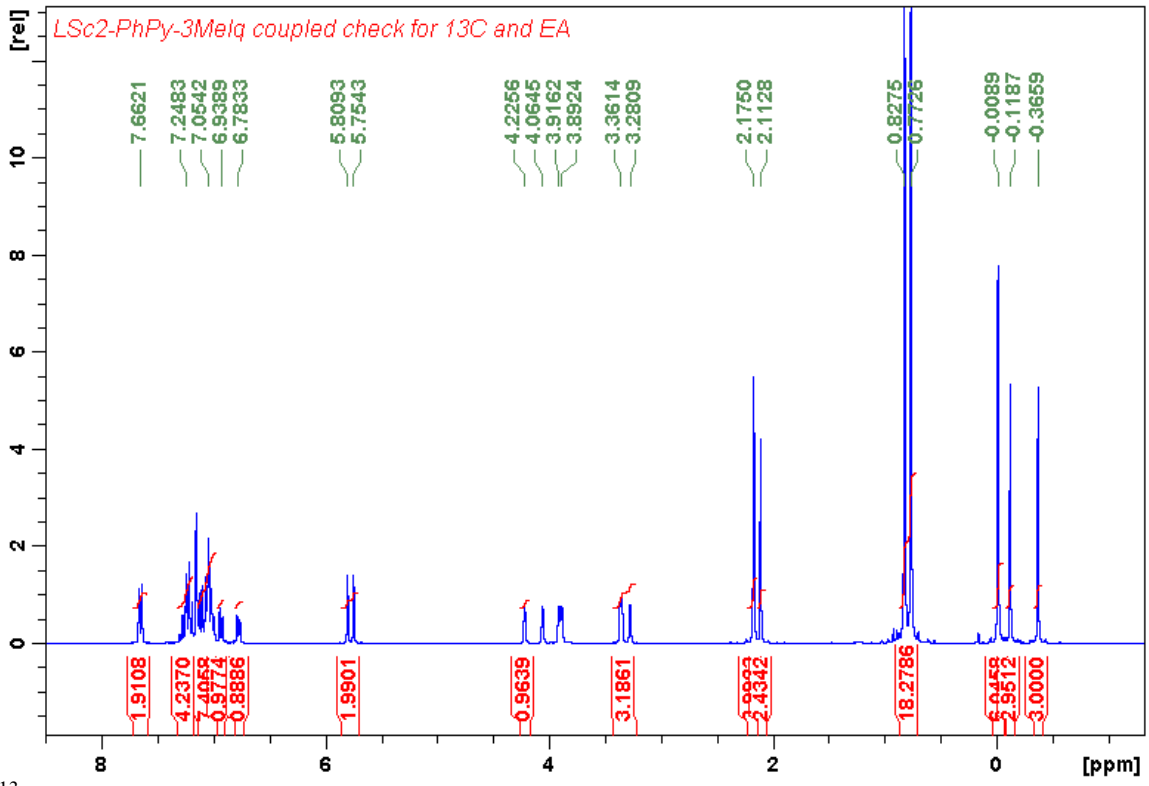


^{13}C NMR (126 mHz, C_6D_6). Solvent peaks for hexanes are present at 32.0, 23.1, and 14.4.

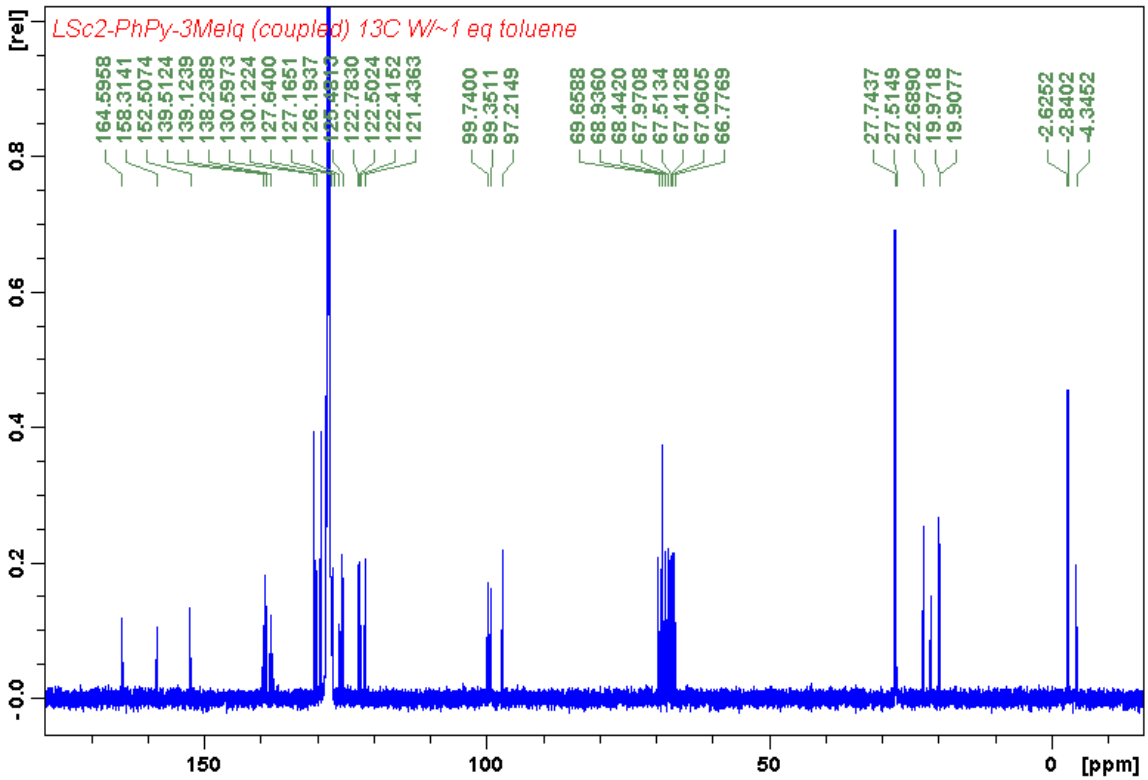


6^{Sc}-py^{Ph}-iqn

^{1}H NMR (500 mHz, C_6D_6):

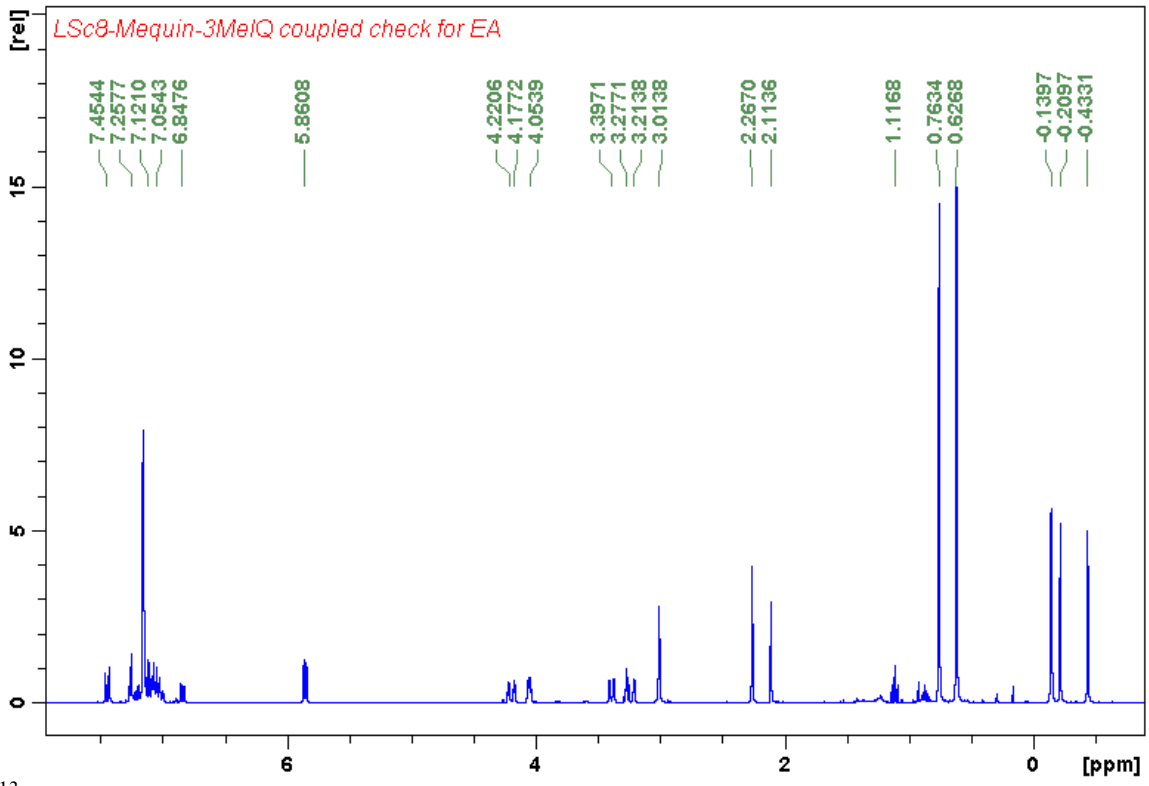


^{13}C NMR (126 mHz, C_6D_6):

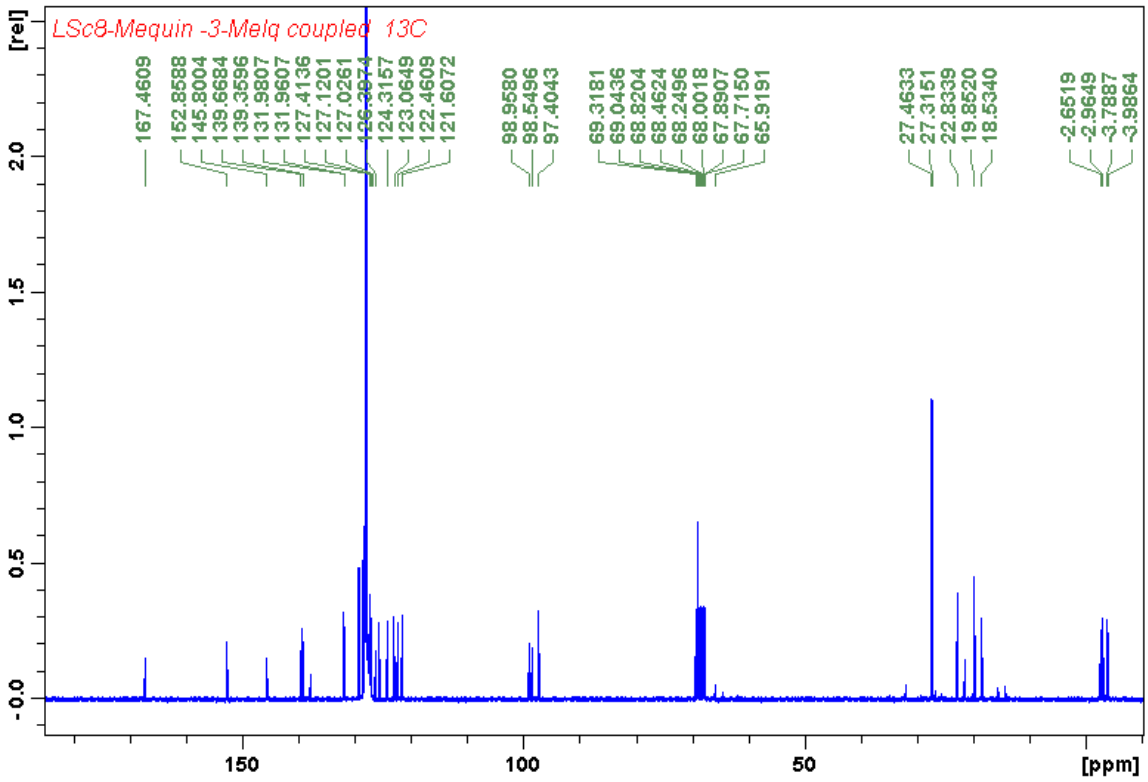


6^{Sc}-qn-iqn

^{1}H NMR (500 mHz, C_6D_6):

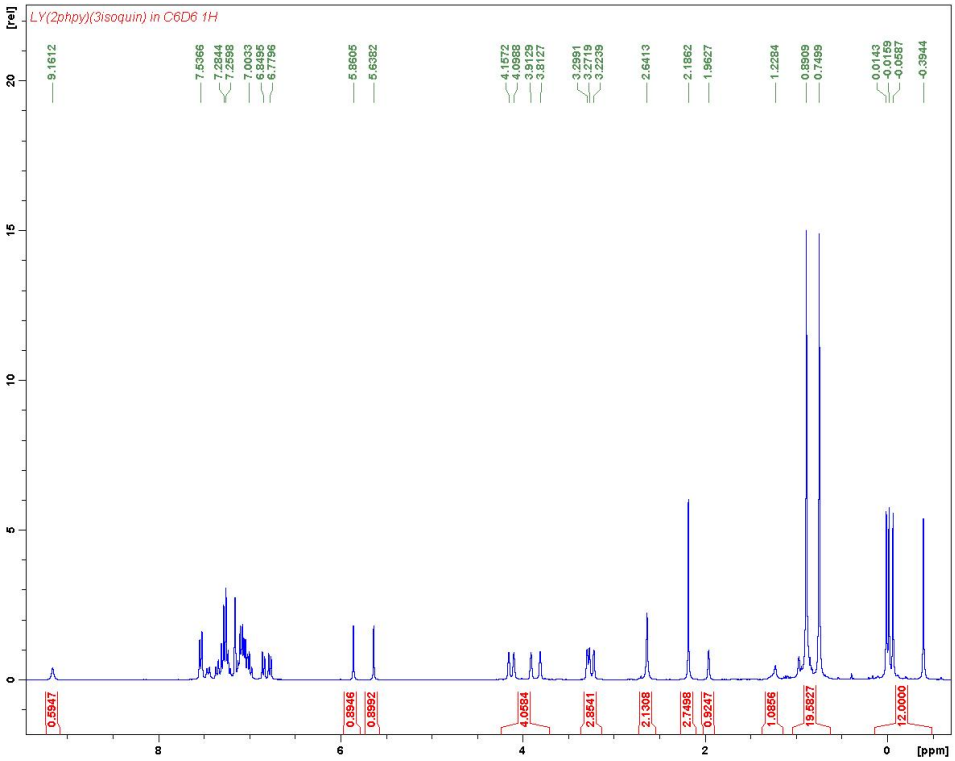


^{13}C NMR (126 mHz, C_6D_6):

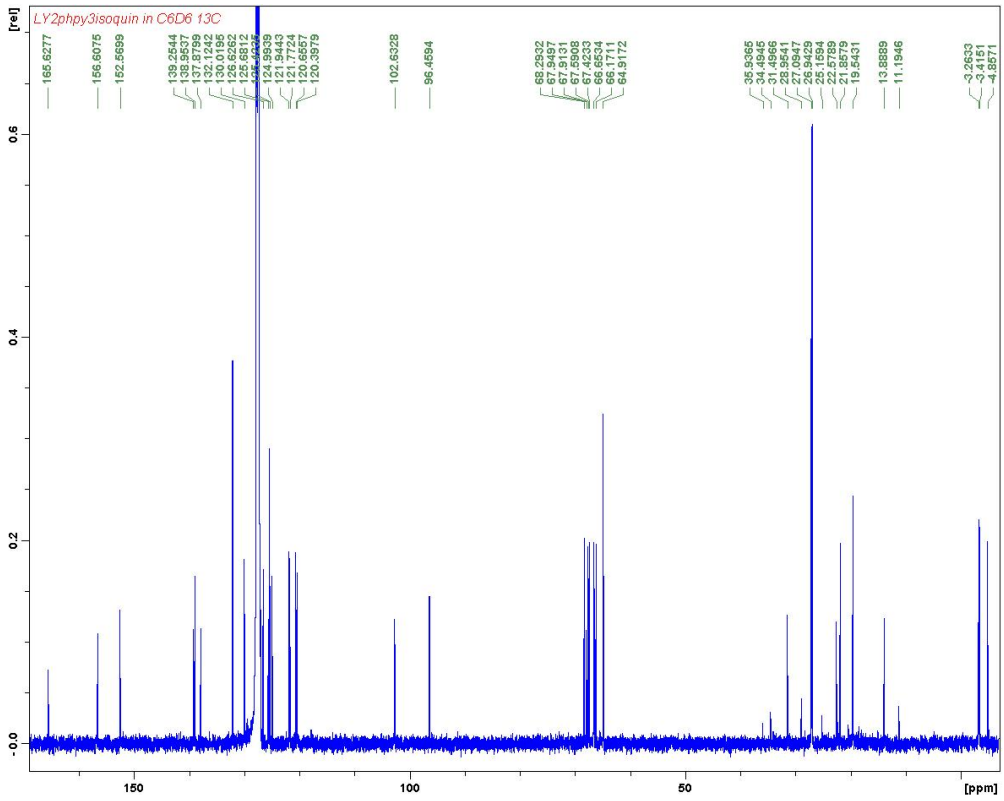


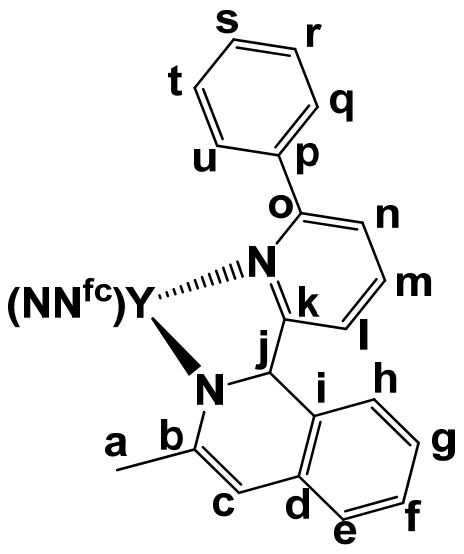
6^{Y}-py^{Ph}-iqn

^{1}H NMR (500 mHz, C_6D_6):

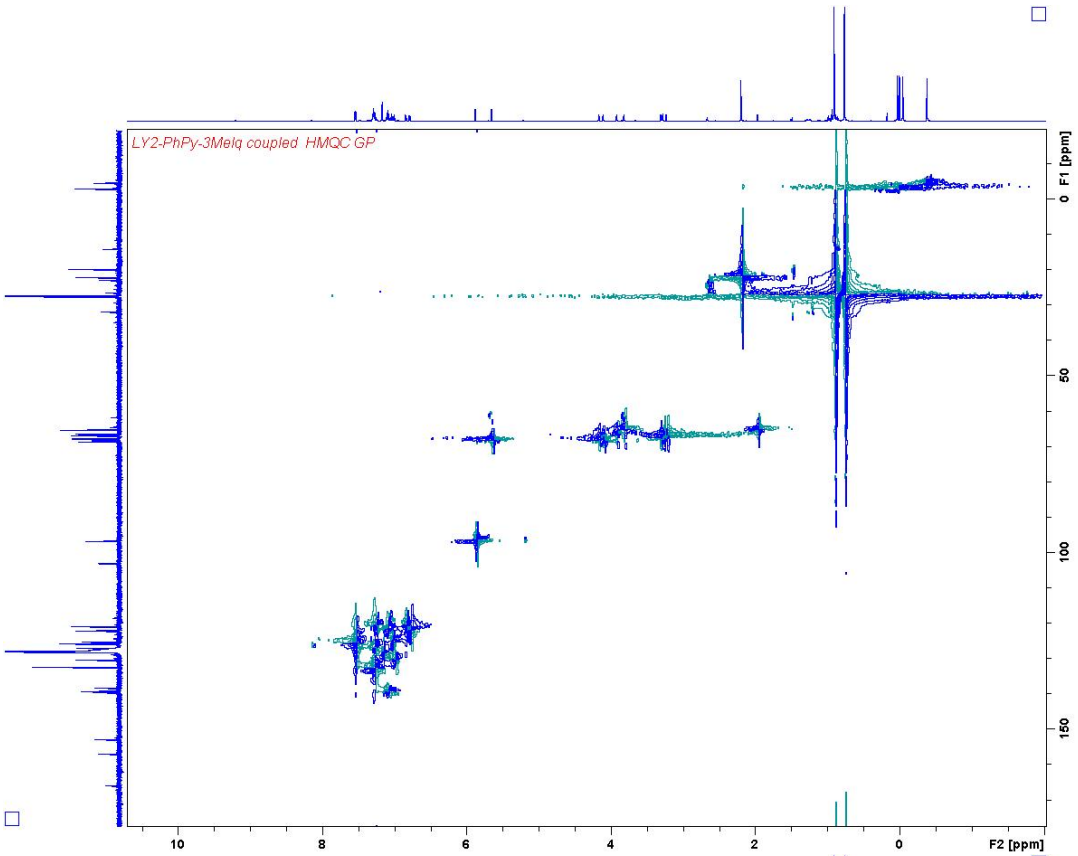


^{13}C NMR (126 mHz, C_6D_6):





^{1}H	^{13}C	Assign.	Primary interactions
2.19	22.2	a	5.88 (j)
--	152.9	b	2.19 (a), 5.65 (c), 5.88 (j)
5.65	68.6	c	7.07 (d)
--	165.9	d	5.65 (c), 6.99 (e, h) 7.08 (f, g),
6.99	120.9	e	7.08 (f, g)
7.08	125.3, 139.3	f, g	5.65 (c), 6.99 (e, h), 5.88 (j)
6.99	130.3	h	7.08 (f, g)
--	165.9	i	5.65 (c), 6.99 (e, h) 7.08 (f, g)
5.88	96.7	j	2.19 (a), 7.28 (m)
--	126.0	k	7.08 (f, g), 7.28 (m)
6.78	120.7	l	6.99 (h) ,7.08 (g), 7.28 (m)
7.28	126.9	m	6.78 (l), 6.83 (n)
6.83	122.0	n	7.28 (m)
--	139.5	o	6.83 (n)
--	156.9	p	6.83 (n), 7.08 (g), 7.53 (q, u)
7.53	125.7, 128.2	q, u	7.28 (r, s, t)
7.28	122.2, 138.2	r, t	6.83 (n), 7.28 (s), 7.53 (q ,u)
7.28	132.4	s	7.28 (r, t)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10
8
6
4
2
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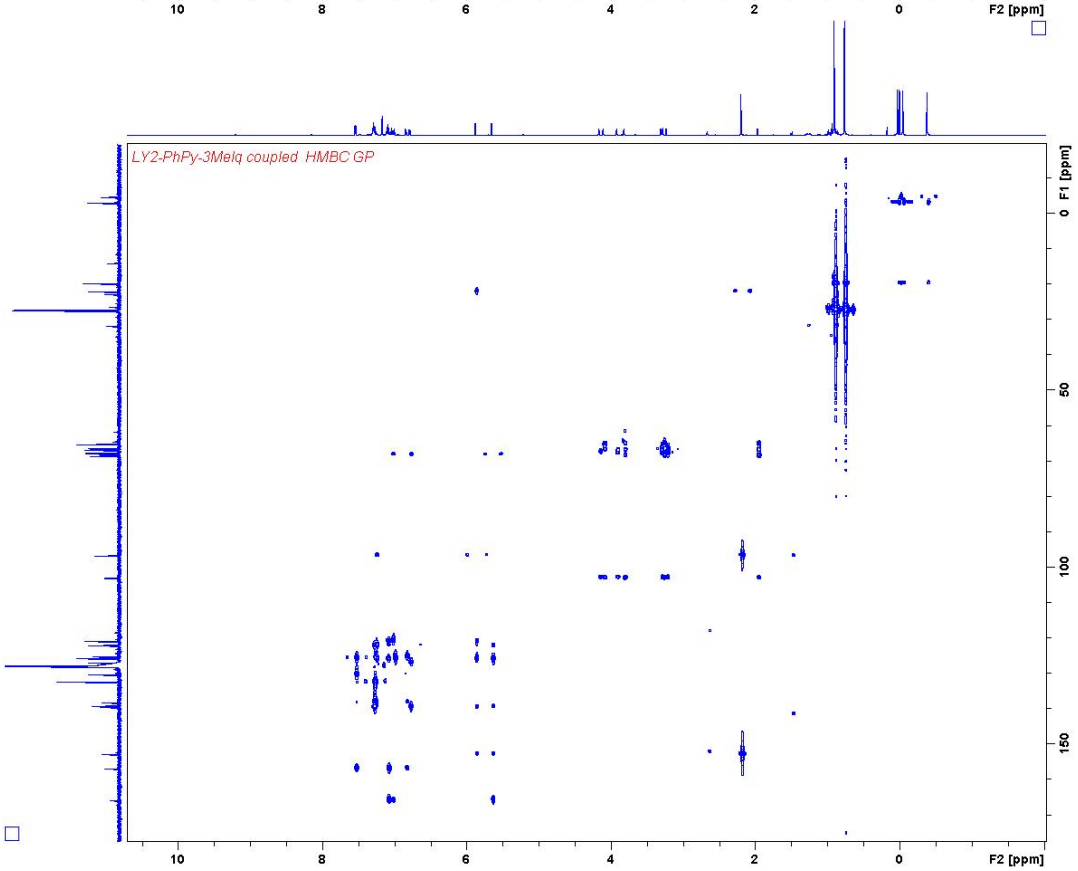
F2 [ppm]


LY2-PhPy-3MeIq coupled HMBC GP
F1 [ppm]
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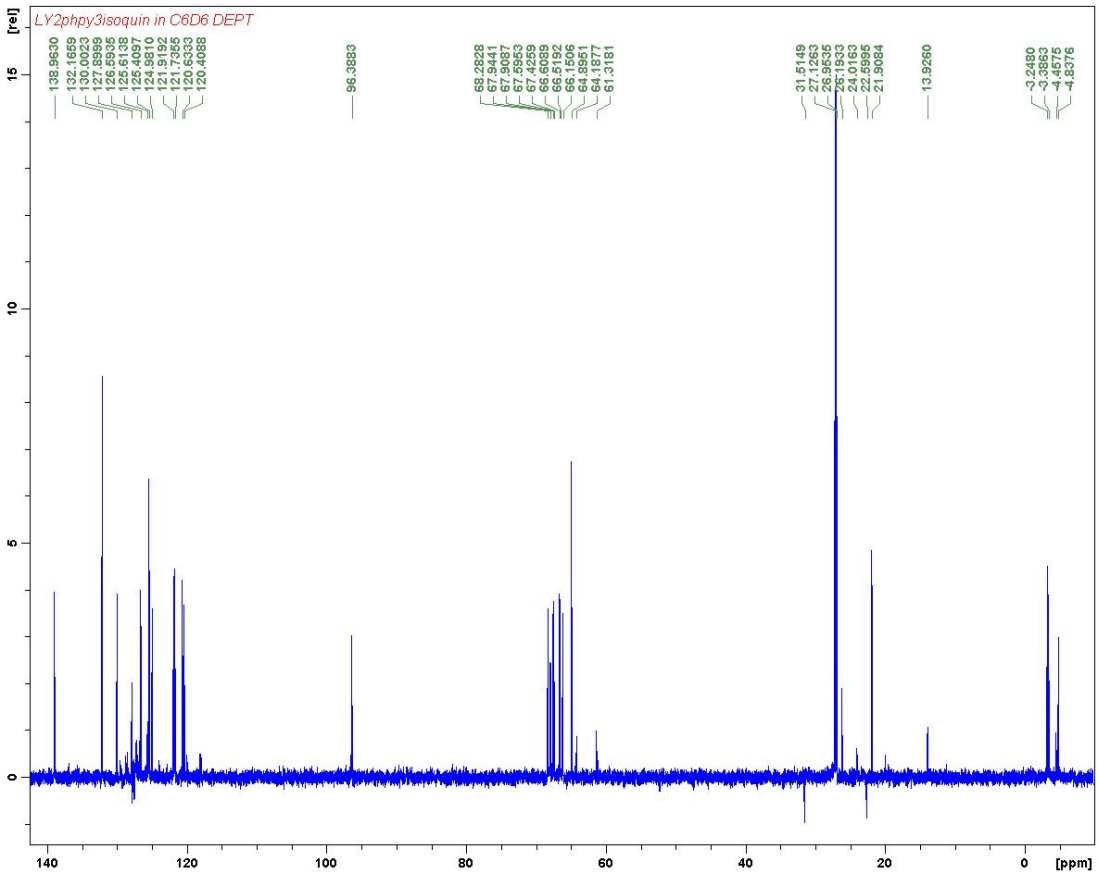
100
150
10
8
6
4
2
0
F2 [ppm]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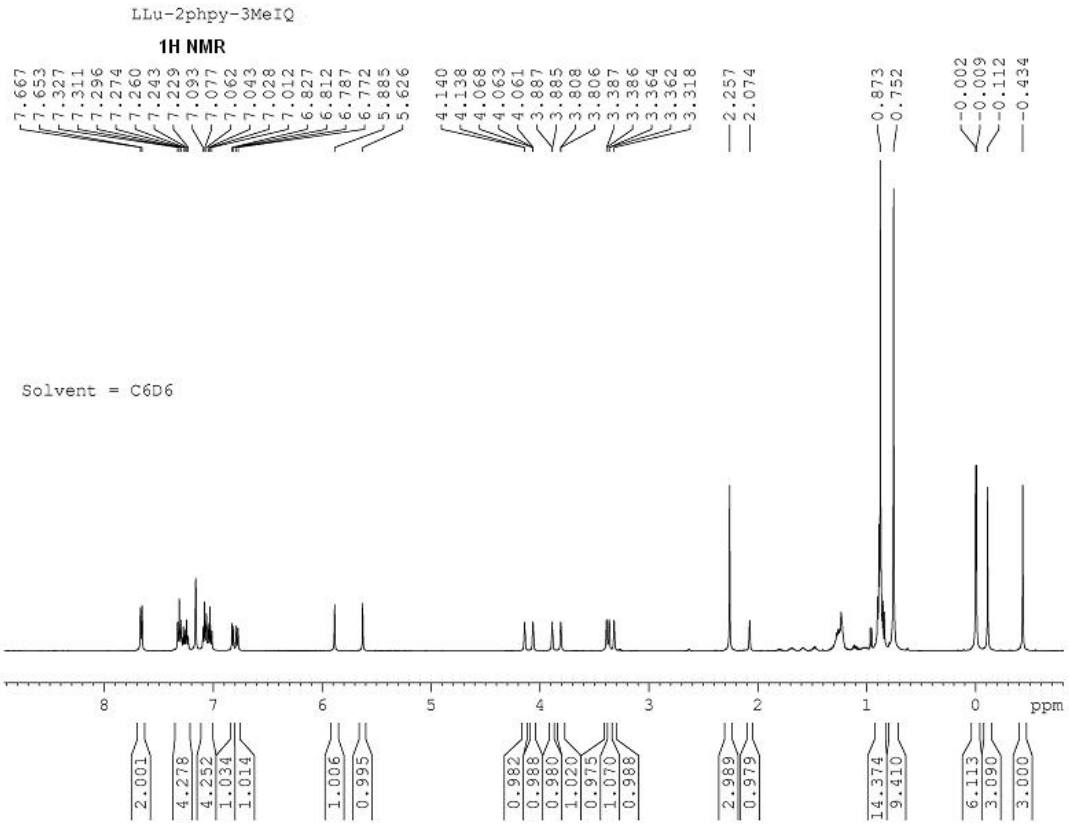
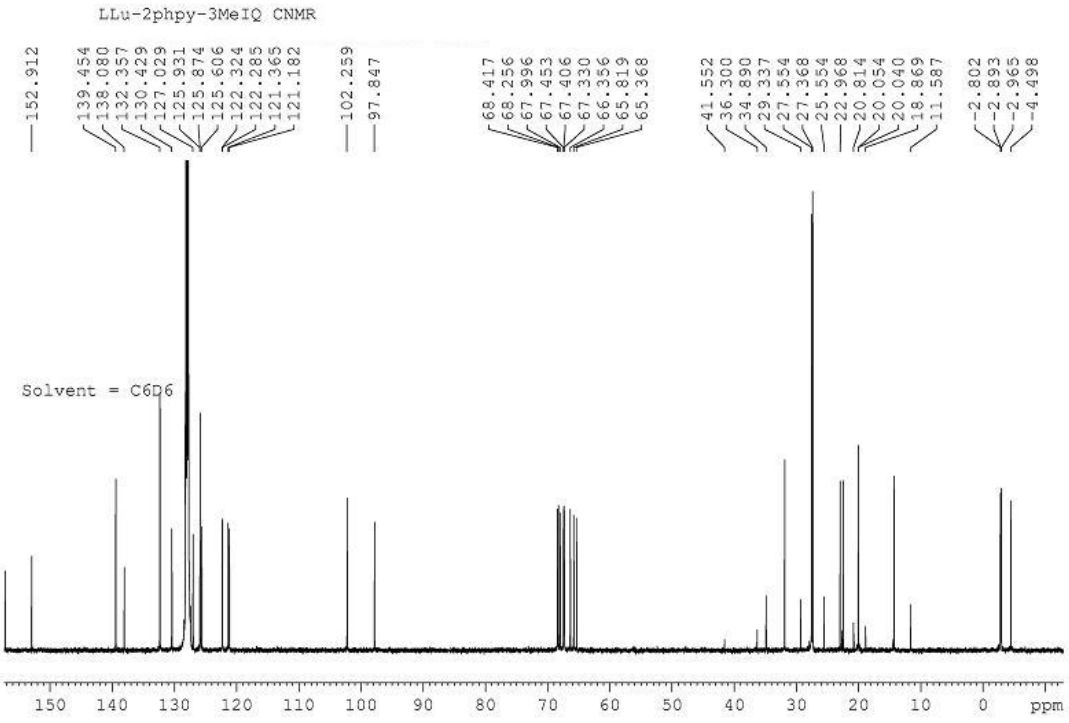
-4.4575
-4.8376
140
120
100
80
60
40
20
0
[ppm]

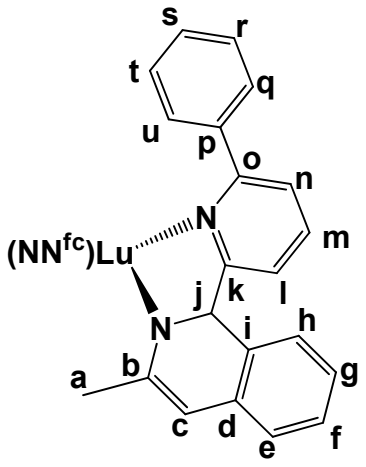
6^{Lu}-py^{Ph}-iqn

^{1}H NMR (500 MHz, C6D6). Solvent peaks for hexanes and pentane are present.

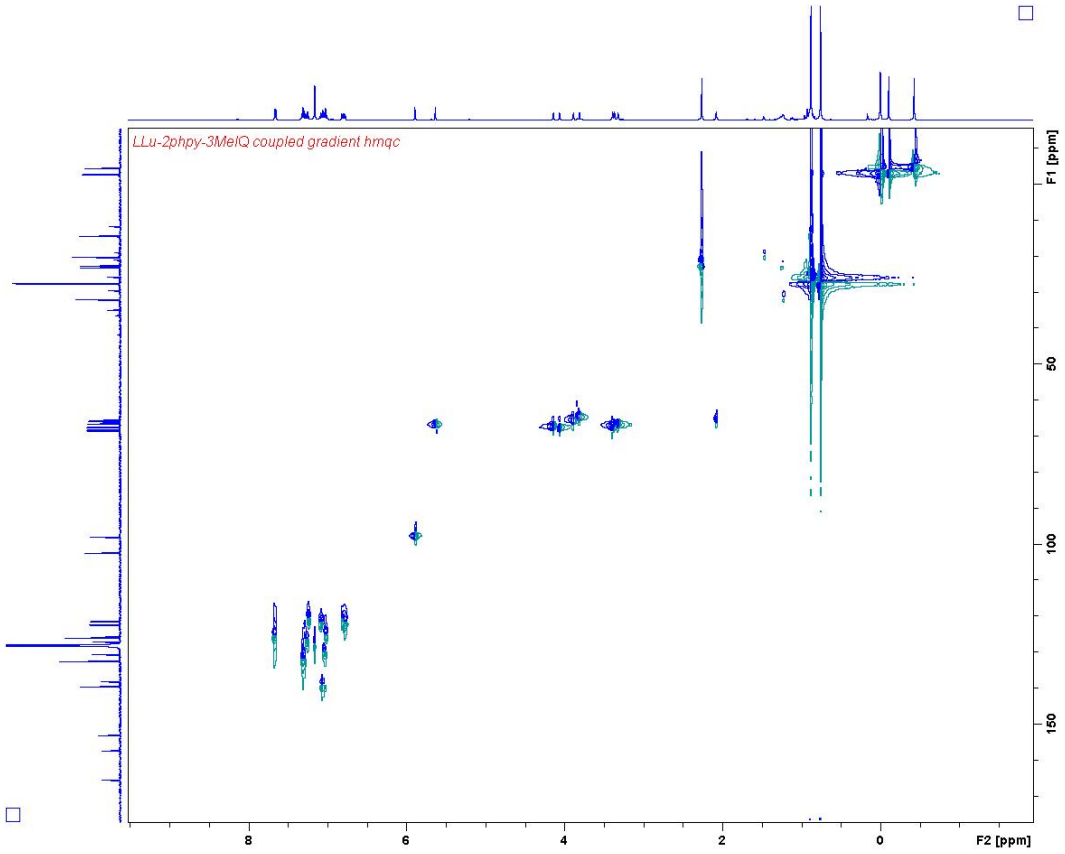


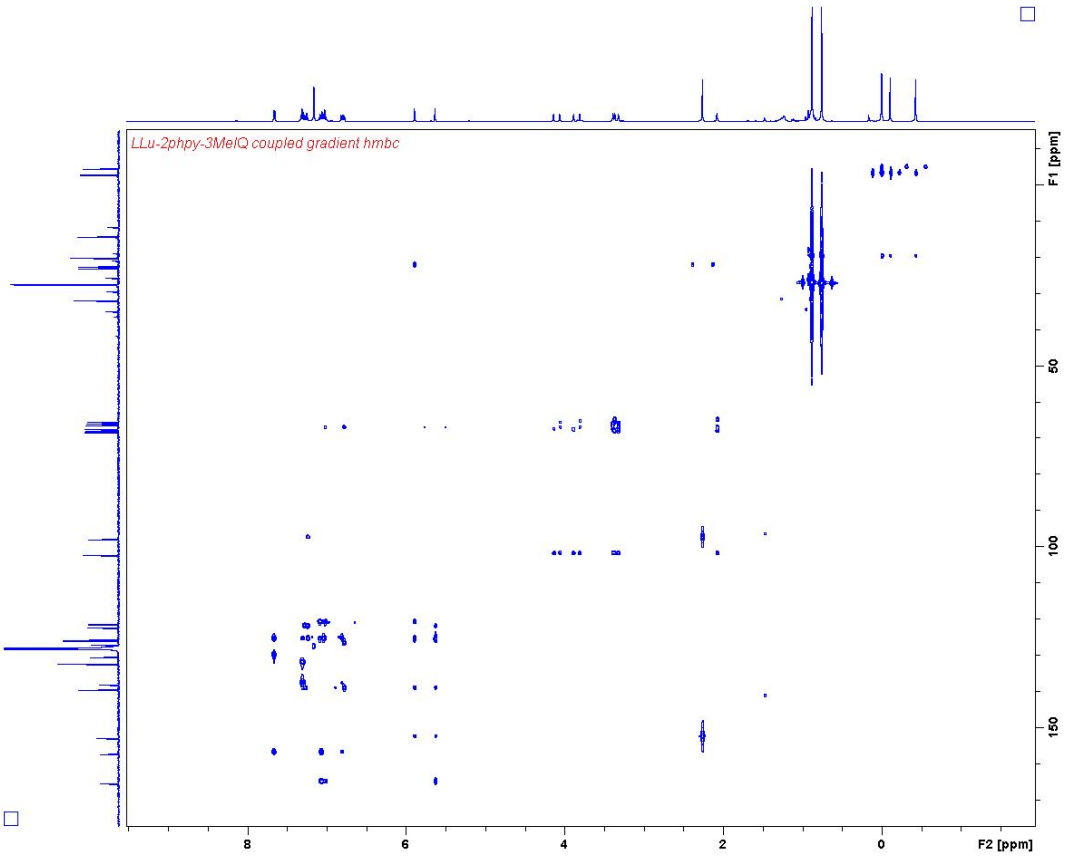
^{13}C NMR (126 MHz, C_6D_6):

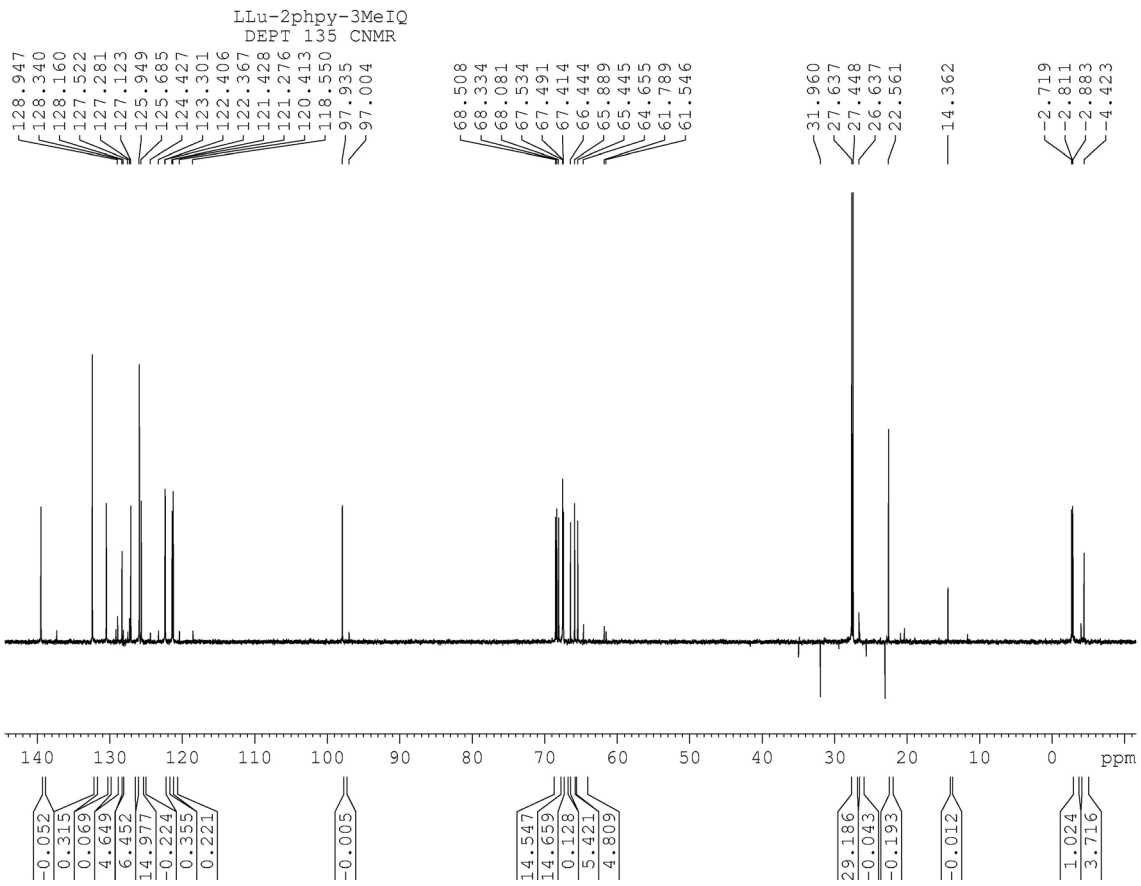




^{1}H	^{13}C	Assign.	Primary interactions (^{1}H)	Primary interactions (^{13}C)	Secondary interactions (^{1}H)	Secondary interactions (^{13}C)
2.26	22.6	a	5.88 (j)	153.0 (b), 97.9 (j)		
--	153.0	b	2.26 (a)	22.6 (a)	5.88 (j)	97.9 (j)
5.63	67.5	c		126.0 (k), 153.0 (b), 165.5 (d, i)	7.08 (n)	122.4 (n)
--	165.5	d	5.63 (c), 7.03 (e), 7.06 (h)	67.5 (c), 125.7 (e), 139.6 (h)		
7.03	125.7	e	6.83, 6.81, 6.78, 6.77 (f,g)	121.5, 122.4 (f,g), 165.5 (d, i)		
6.83, 6.81, 6.78, 6.77	121.5, 122.4	f, g	7.03 (e), 7.26, 7.27 (l)	125.7 (e), 127.1 (l)		157.3 (o)
7.07	139.6	h	none	157.3 (o), 165.5 (d, i)		
--	165.5	i	5.63 (c), 7.03 (e), 7.06 (h)	67.5 (c), 125.7 (e), 139.6 (h)		
5.88	97.9	j	2.28 (a)	22.6 (a), 126.0 (k)	7.24 (m)	153.0 (b), 121.3 (m)
--	126.0	k	5.63 (c), 5.88 (j)	67.5 (c), 97.9 (j)		
7.26, 7.27	127.1	l	6.83, 6.81, 6.78, 6.77 (f,g), 7.08 (n)	121.5, 122.4 (f,g) 122.4 (n)		
7.24	121.3	m	7.08 (n), 7.67, 7.65 (r,t)	122.4 (n), 126.0 (r,t)	5.88 (j)	97.9 (j)
7.08	122.4	n	7.26, 7.27 (l), 7.24 (m)	127.1 (l), 121.3 (m)	5.63 (c)	67.5 (c)
--	157.3	o	7.67, 7.65 (r,t), 7.07 (h)	126.0 (r,t), 139.5 (h)	6.83, 6.81, 6.78, 6.77 (f,g)	121.5, 122.4 (f,g)
--	138.2	p	7.31 (q,u)	132.5 (q,u)		
7.31	132.5	q, u		138.2 (p)		
7.67, 7.65	126.0	r, t	7.04 (s)	157.3 (o), 130.5 (s)		
7.04	130.5	s	7.67, 7.65 (r,t)	126.0 (r,t)		

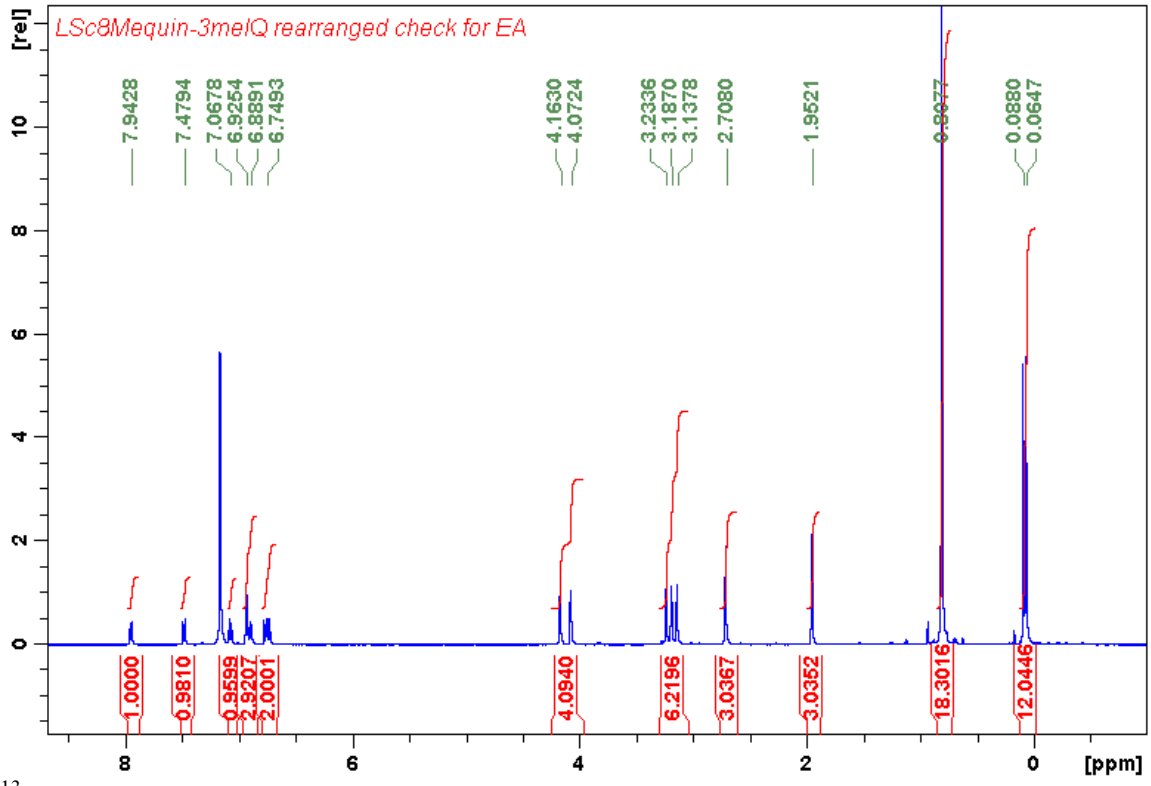

LLu-2phpy-3MeIQ coupled gradient hmqc
F1 [ppm]
50
100
150
8
6
4
2
0
F2 [ppm]


LLu-2phpy-3MeIQ coupled gradient hmbc
F1 [ppm]
50
100
150
8
6
4
2
0
F2 [ppm]

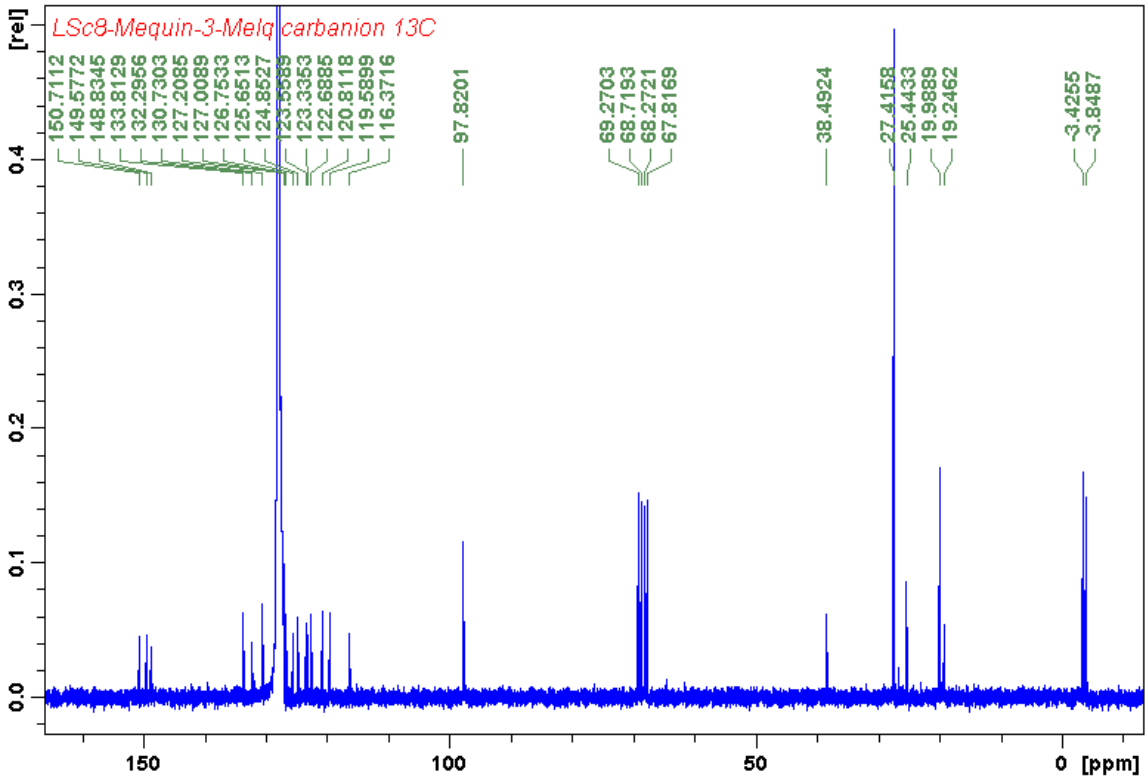

LLu-2phpy-3MeIQ
DEPT 135 CNMR
128.947
128.340
128.160
127.522
127.281
127.123
125.949
125.685
124.427
123.301
122.406
122.367
121.428
121.276
120.413
118.550
97.935
97.004
68.508
68.334
68.081
67.534
67.491
67.414
66.444
65.889
65.445
64.655
61.789
61.546
31.960
27.637
27.448
26.637
22.561
14.362
-2.719
-2.811
-2.883
-4.423
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
-0.052
0.315
0.069
4.649
6.452
14.977
-0.224
0.355
0.221
-0.005
14.547
14.659
0.128
5.421
4.809
29.186
-0.043
-0.193
-0.012
1.024
3.716

7^{Sc}-qn-iqn

^{1}H NMR (500 mHz, C_6D_6):



^{13}C NMR (126 mHz, C_6D_6):

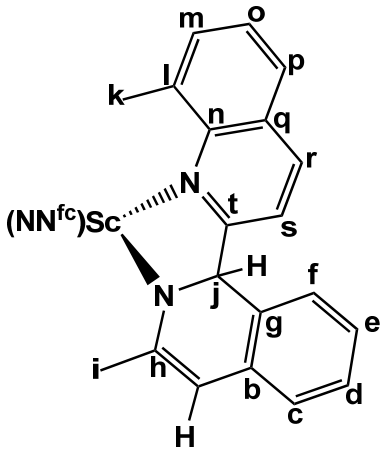


NMR experiments

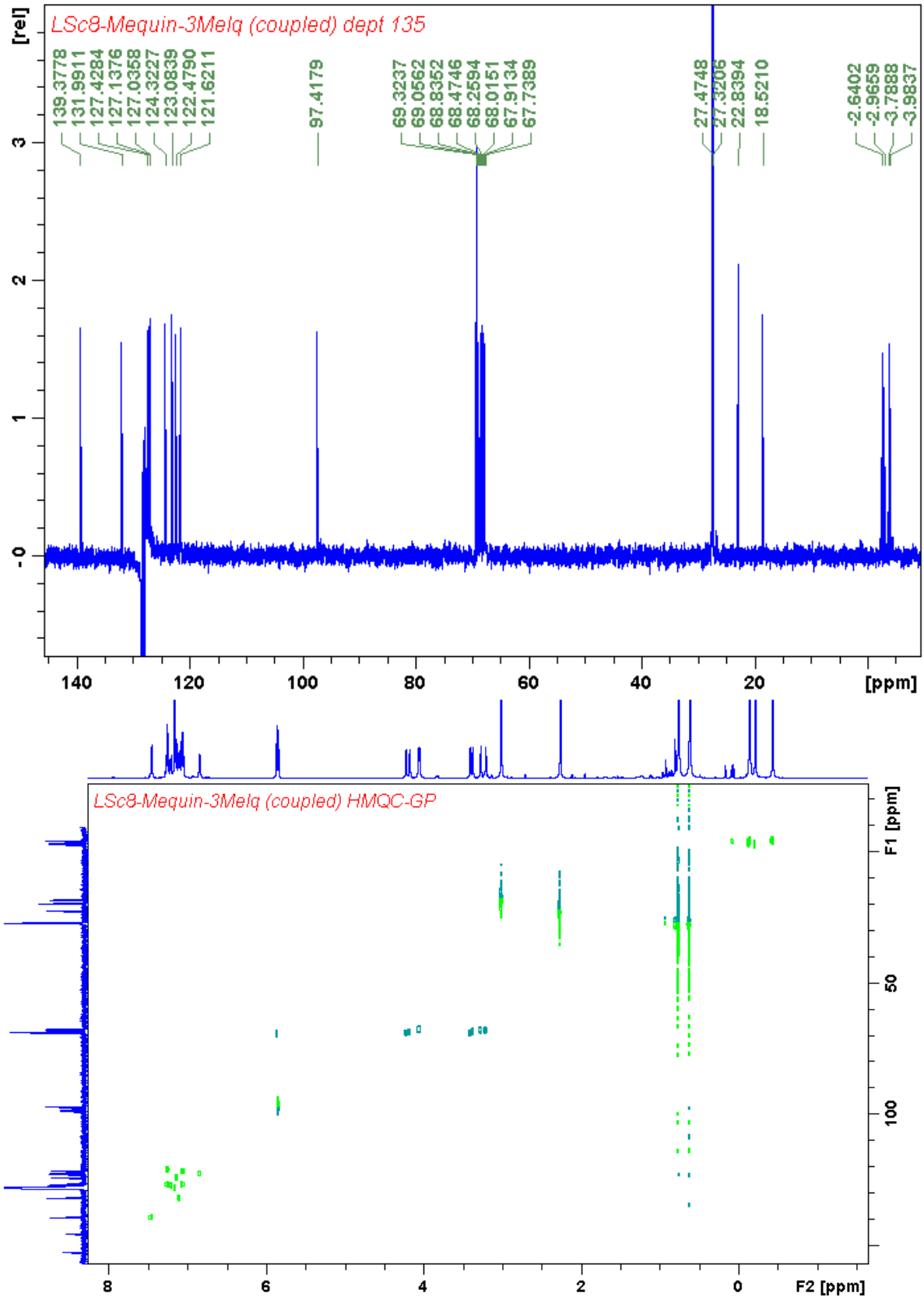
6^{Sc}-qn-iqn

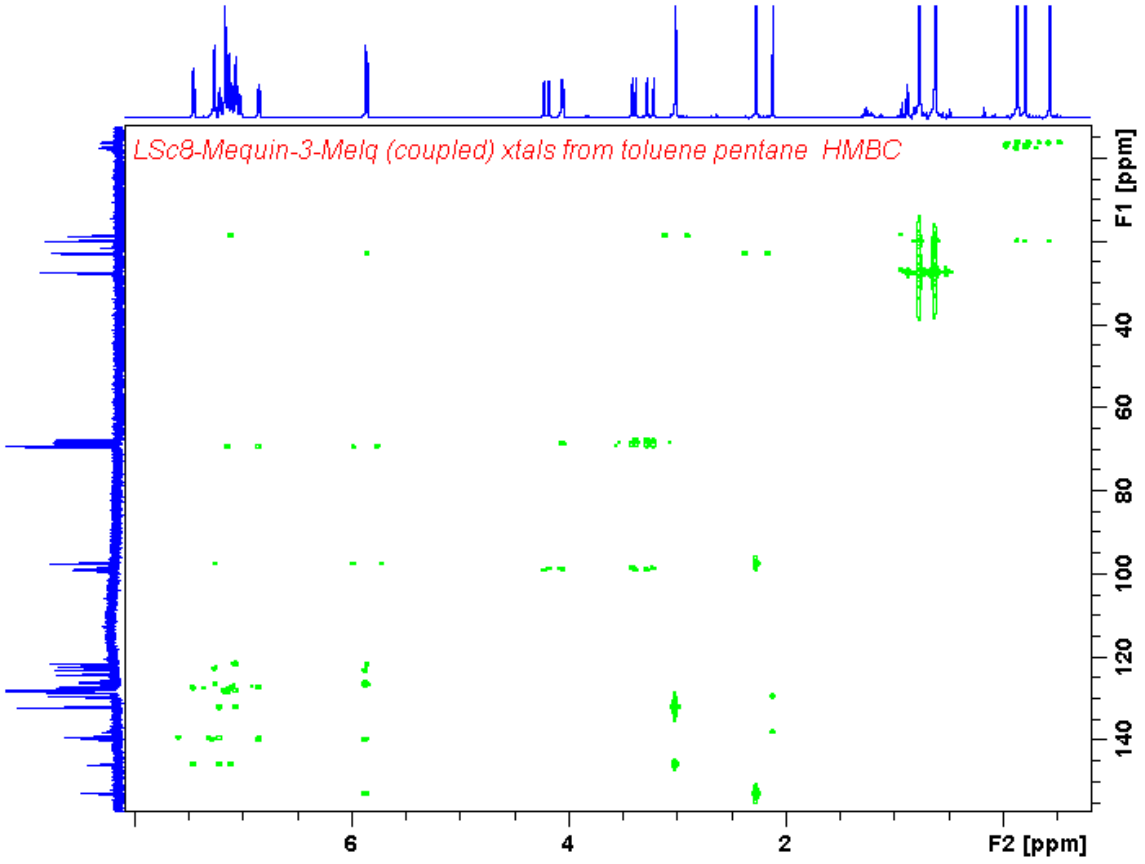
Dept 135 NMR (126 MHz, C_6D_6) shows no methylene carbon resonance and ten quaternary carbon resonances at δ (ppm): 167.4 (t), 152.8 (h), 145.8 (l), 139.7 (b or g), 127.5 (q or n), 126.4 (b or g), 99.0 (fc-*C*-N), 98.5 (fc-*C*-N), 19.9 (Si*C*$(CH_3)_3$), and 19.8 (Si*C*$(CH_3)_3$).

Gradient pulse HMQC and HMBC experiments were complicated by extensive cross-ring coupling of ^{1}H and ^{13}C resonances that made unambiguous assignment of the spectra difficult. The assignments shown below are based on the strongest interactions observed in the spectra.



^{1}H	^{13}C	Assign.	Primary interaction
5.84	97.4	a	7.25, 2.26 (i)
No	139.7	b or g	7.26, 6.85 (f), 5.86 (j)
7.13	124.3	c	Nothing
7.25	121.6	d	7.06 (o)
7.26	127.1	e	6.85 (f)
6.85	123.1	f	5.86 (j), 7.26
No	126.4	b or g	7.26, 5.86 (j) 5.84 (a)
No	152.8	h	5.84 (a), 2.26 (i)
2.26	22.8	i	5.84 (a)
5.86	69.3	j	7.13 (c)
3.01	18.5	k	7.10 (m)
No	145.8	l	7.45 (s), 7.20 (r), 7.10 (m), 3.01 (k)
7.11	132.0	m	3.01 (k), 7.20 (r), 7.06 (o)
7.06	122.5	o	7.25
No	132.0	q or n	3.01 (k), 7.20 (r), 7.06 (o)
7.21	127.4	r	7.45 (s)
7.45	139.3	s	7.26, 6.84 (f), 5.86 (j)
No	167.4	t	Nothing


LSc8-Mequin-3Melq (coupled) dept 135
[rel]
3
2
1
-0
139.3778
131.9911
127.4284
127.1376
127.0358
124.3227
123.0839
122.4790
121.6211
97.4179
69.3237
69.0562
68.8352
68.4746
68.2594
68.0151
67.9134
67.7389
27.4748
27.3206
22.8394
18.5210
-2.6402
-2.9659
-3.7888
-3.9837
140
120
100
80
60
40
20
[ppm]
LSc8-Mequin-3Melq (coupled) HMQC-GP
F1 [ppm]
50
100
8
6
4
2
0
F2 [ppm]

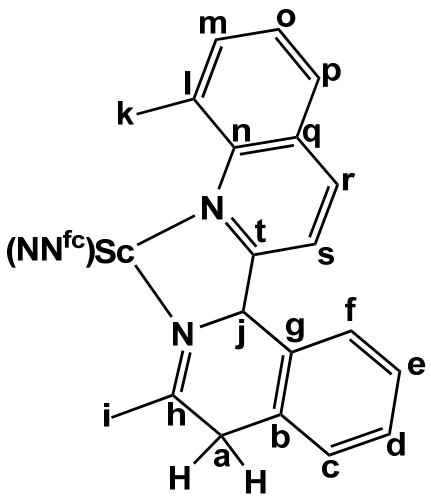

LSc8-Mequin-3-Melq (coupled) xtals from toluene pentane HMBC
F1 [ppm]
40
60
80
100
120
140
6
4
2
F2 [ppm]

7^{Sc}-qn-iqn

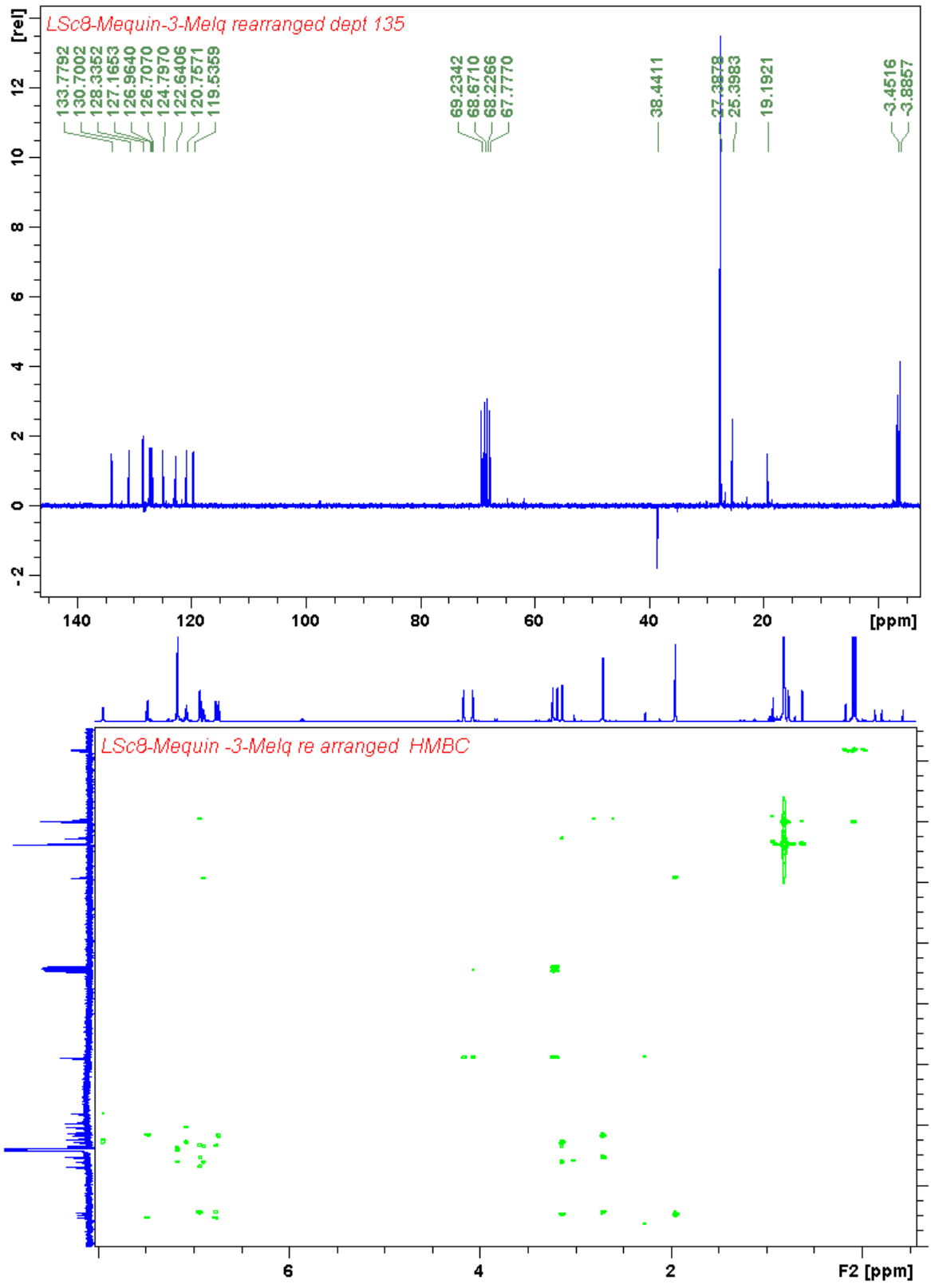
Dept 135 NMR (126 MHz, C_6D_6) shows only 1 methylene carbon resonance at δ = 38.5 ppm and nine quaternary carbon resonances at δ = 150.7 (t), 149.6 (h), 148.8 (l), 132.3 (g), 125.7 (b), 123.6 (l), 123.3 (q), 116.4 (j), 97.8 (fc-*C*-N), and 19.9 (Si*C*$(CH_3)_3$).

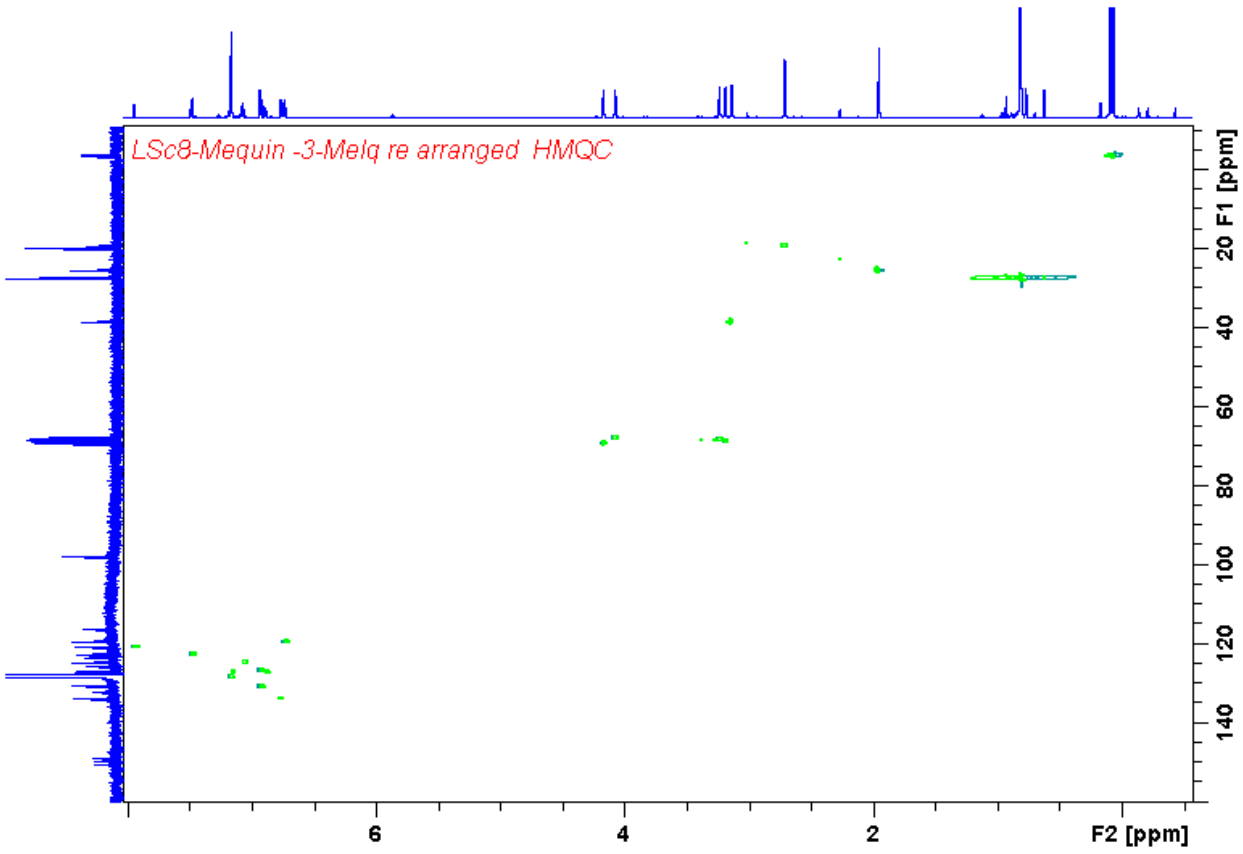
Gradient pulse HMQC, and HMBC

Gradient pulse HMQC and HMBC NMR experiments were complicated by extensive cross-ring coupling of ^{1}H and ^{13}C resonances that made unambiguous assignment of the spectra difficult. The assignments shown below are based on the strongest interactions observed in the spectra.



^{1}H	^{13}C	Assign.	Primary interaction	Secondary interaction
3.13	38.5	a	6.89 (f), 1.94 (i)	7.94 (c)
No	125.6	b	7.07 (d), 3.13 (a)	7.94 (c),
7.94	120.8	c	7.07 (d)	7.17 (e)
7.07	124.8	d	7.94 (c)	7.17(e)
7.17	127.0	e	6.89 (f)	
6.89	127.2	f	3.13 (a)	
No	132.3	g	6.89 (d), 3.13 (a)	
No	149.6	h	1.94 (i)	
1.94	25.5	i	3.13(a)	
No	116.4	j	3.13 (a)	
2.71	19.23	k	6.92 (p or m)	
No	123.5	l	6.73 (o), 2.71 (k)	
6.92	130.7	m	6.92 (p), 2.71 (k)	
No	148.8	n	6.92, 2.71 (k)	
6.73	119.6	o	Nothing	
6.92	126.7	p	6.92 (m)	
No	123.31	q	7.49 (r)	
7.49	122.7	r	Nothing	
6.76	133.8	s	6.92 (m)	
No	150.6	t	7.49 (r), 6.73 (o), 6.76 (s)	

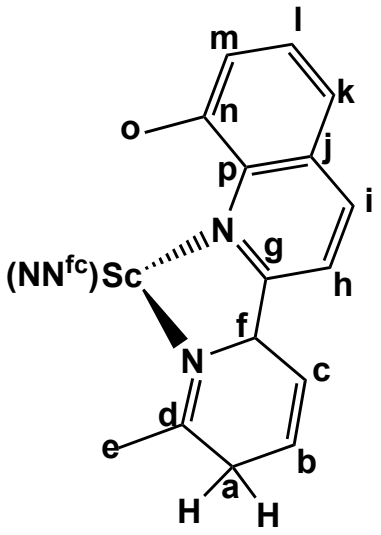

LSc8-Mequin-3-Melq rearranged dept 135
[rel]
133.7792
130.7002
128.3352
127.1653
126.9640
126.7070
124.7970
122.6406
120.7571
119.5359
69.2342
68.6710
68.2266
67.7770
38.4411
27.3878
25.3983
19.1921
-3.4516
-3.8857
[ppm]
LSc8-Mequin -3-Melq re arranged HMBC
F1 [ppm]
F2 [ppm]


LSc8-Mequin -3-Melq re arranged HMQC
F1 [ppm]
20
40
60
80
100
120
140
6
4
2
F2 [ppm]

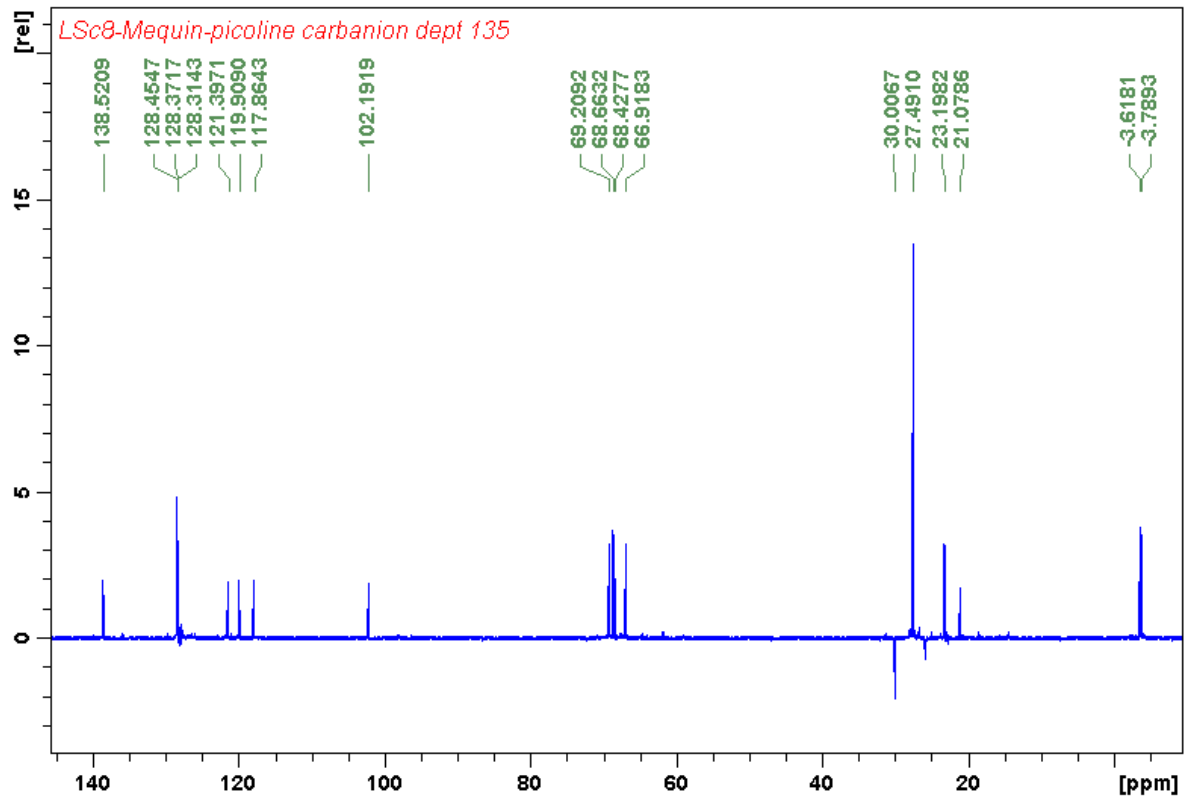
7^{Sc}-qn-pic

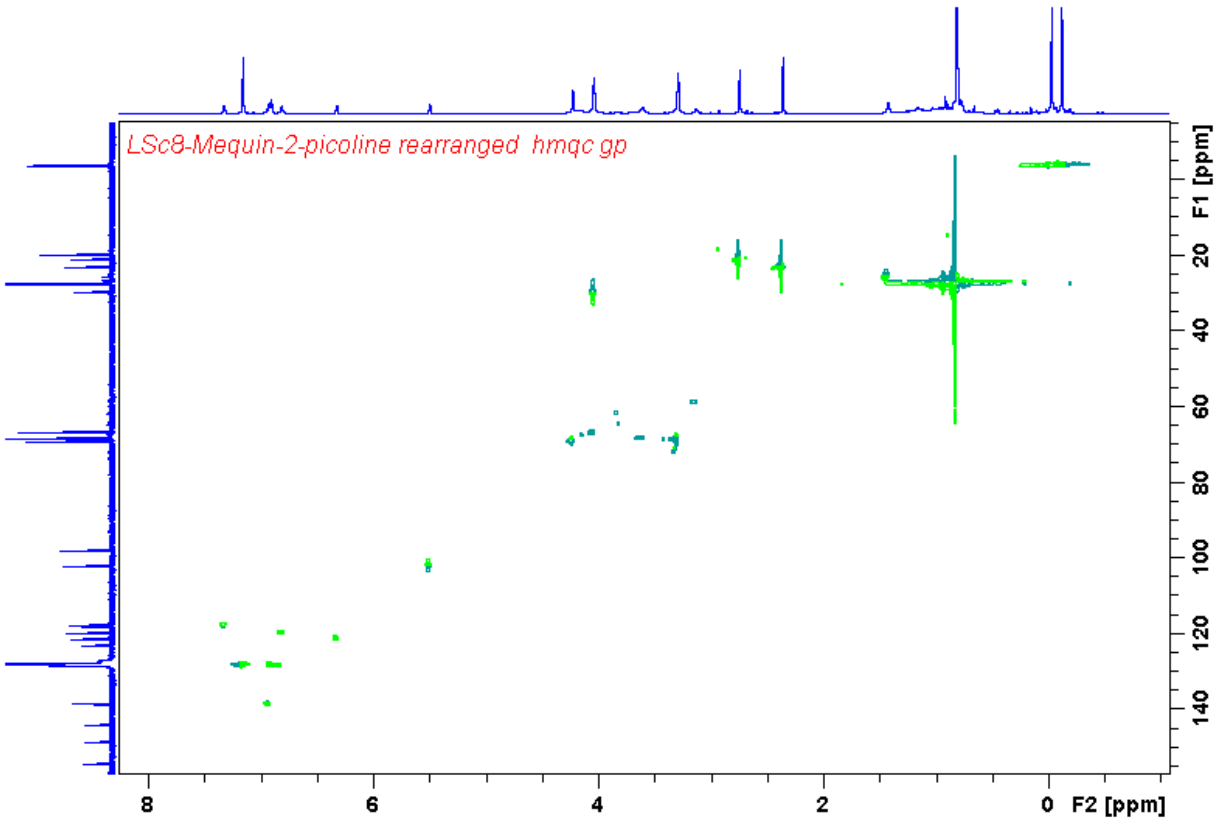
Dept 135 NMR (150 MHz, C_6D_6) shows only 1 methylene carbon resonance at δ (ppm): 30.0 and eight quaternary carbon resonances at 159.4 (g), 154.4 (n), 148.6 (d), 144.0 (p or j), 123.2 (p or j), 118.3 (f), 98.1 (fc-*C*-N), and 19.9 (Si*C*$(CH_3)_3$).

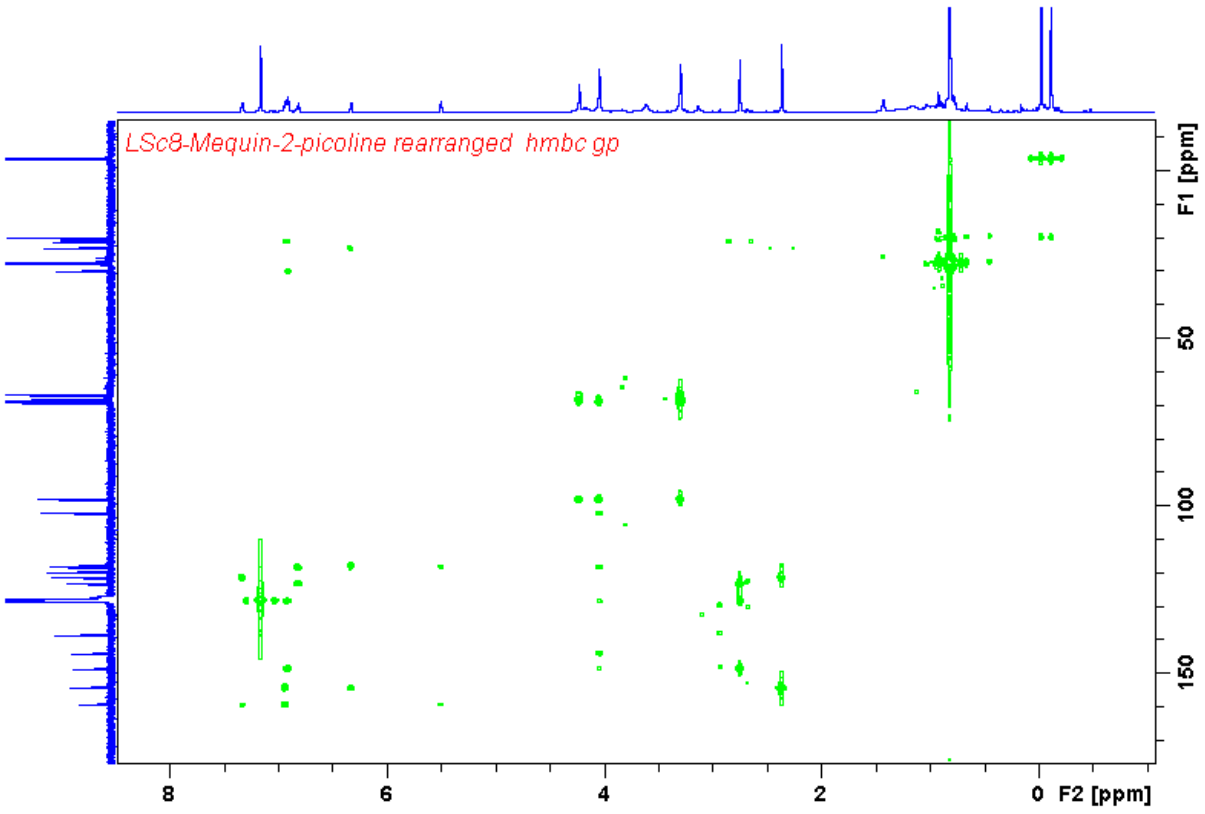
Gradient pulse HMQC and HMBC experiments were complicated by extensive cross-ring coupling of ^{1}H and ^{13}C resonances that made unambiguous assignment of the spectra difficult. The assignments shown below are based on the strongest interactions observed in the spectra.



^{1}H	^{13}C	Assign.	Primary interaction	Secondary interaction
4.04	30.02	a	5.50 (b),	6.91 (k or m)
5.50	102.2	b	4.04 (a)	
6.91	128.35	c	2.75 (e)	4.04(a)
No	148.6	d	6.91 (c), 2.74 (a)	
2.75	21.1	e	6.91 (c)	
No	118.3	f	4.04 (a)	
No	159.4	g	5.50 (b), 6.93 (a), 7.33 (h)	
7.33	117.8	h	6.33, 2.37(0)	
6.33	121.4	i, k, l, or m	7.33 (h), 2.36 (h)	
No	123.3	p or j	3.13 (a)	
No	144.0	p or j	4.04 (a)	
6.93	138.51	i, k, l, or m	6.33	
6.81	119.9	i, k, l, or m	nothing	
6.93	128.46	i, k, l, or m	6.93	
No	154.4	n	6.93, 6.32, 2.36(o)	
2.36	23.2	o	6.32	

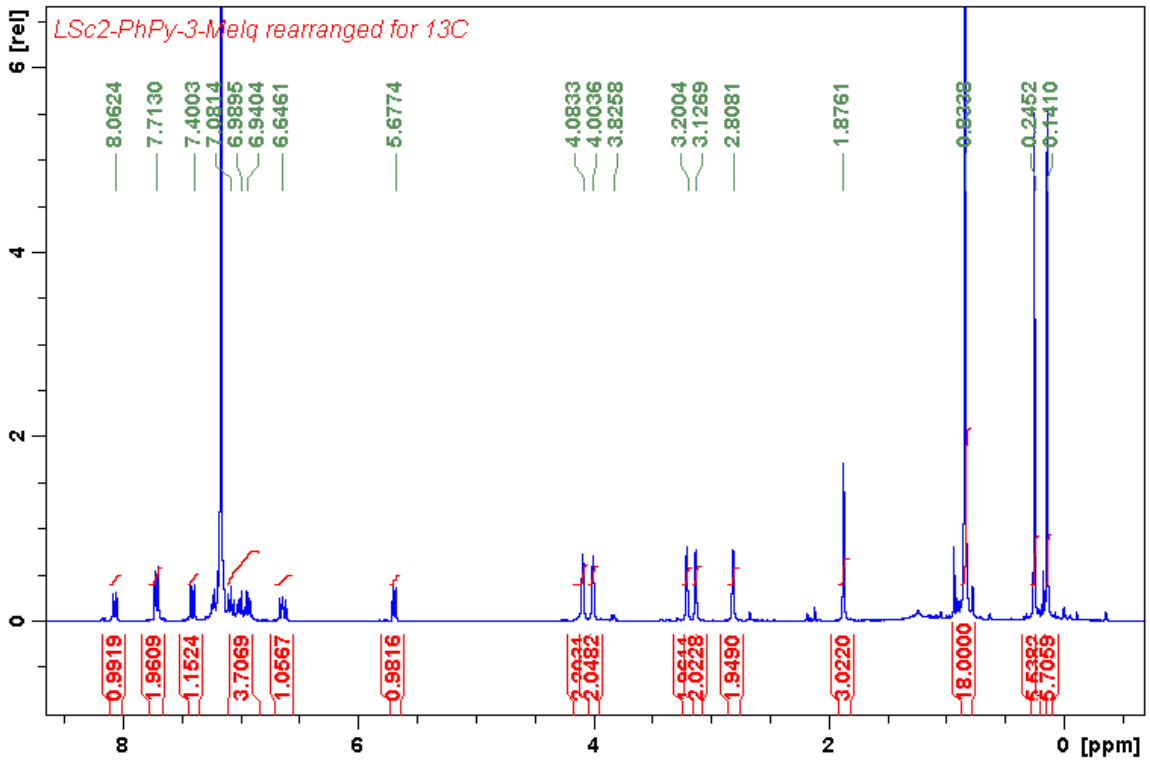

LSc8-Mequin-picoline carbanion dept 135
[rel]
138.5209
128.4547
128.3717
128.3143
121.3971
119.9090
117.8643
102.1919
69.2092
68.6632
68.4277
66.9183
30.0067
27.4910
23.1982
21.0786
-3.6181
-3.7883
[ppm]


LSc8-Mequin-2-picoline rearranged hmqc gp
F1 [ppm]
F2 [ppm]

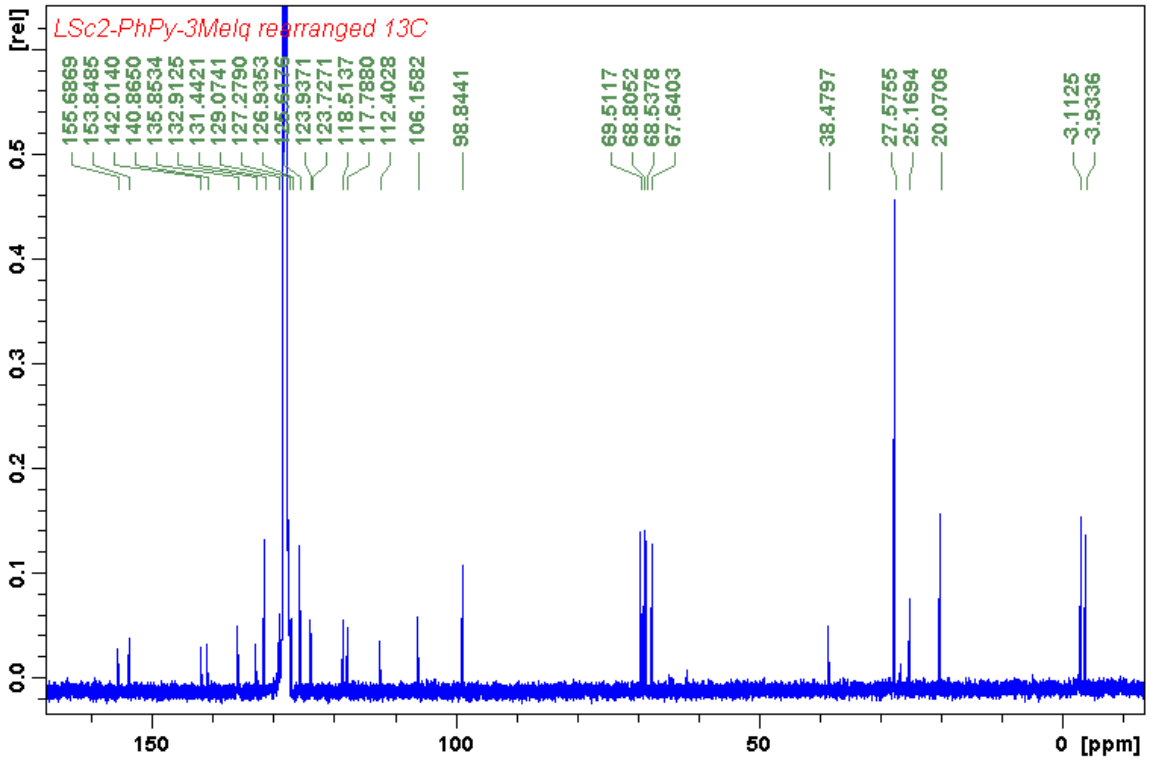

LSc8-Mequin-2-picoline rearranged hmbc gp
F1 [ppm]
50
100
150
8
6
4
2
0 F2 [ppm]

7^{Sc}-py^{Ph}-iqn

^{1}H NMR (600 MHz, C_6D_6):

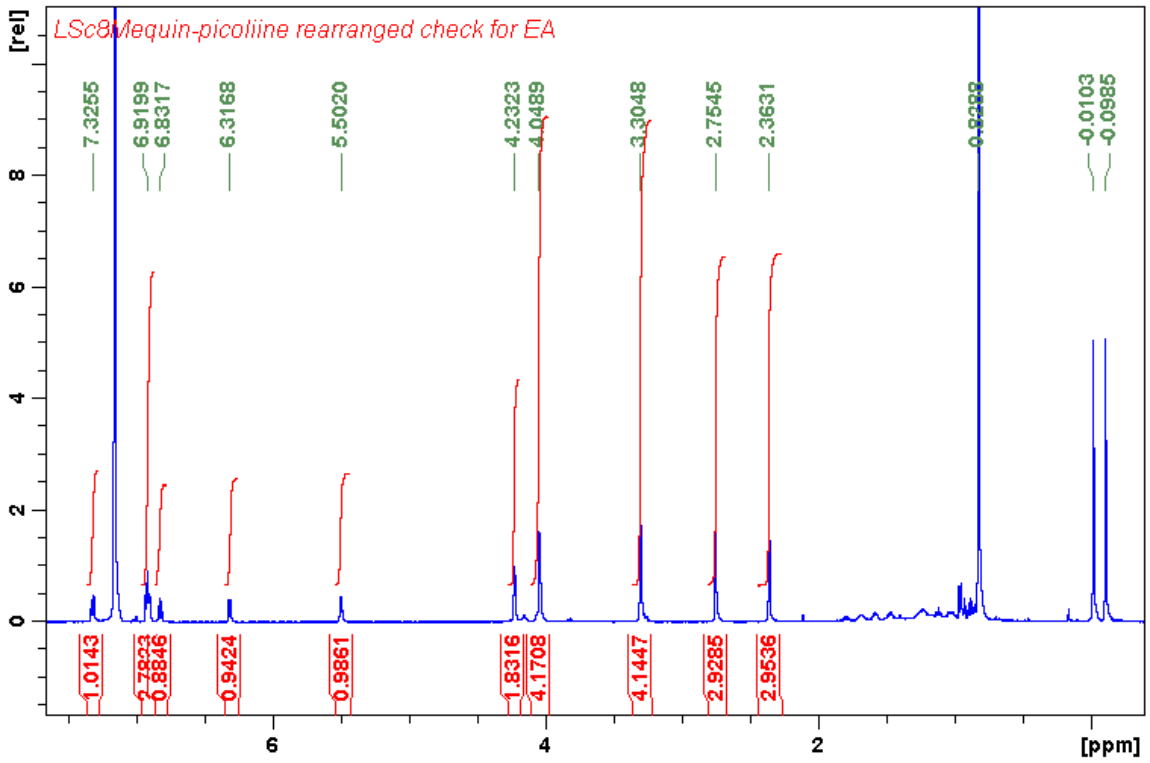


^{13}C NMR (151 mHz, C_6D_6):

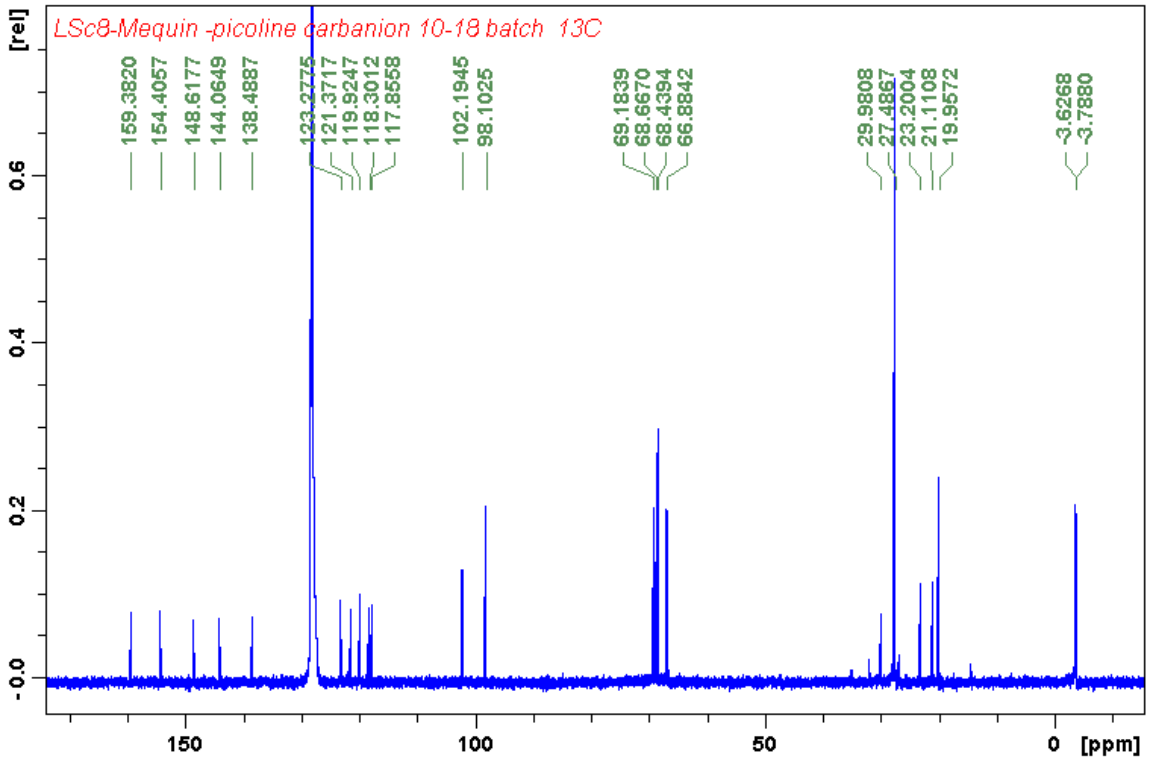


7^{Sc}-qn-pic

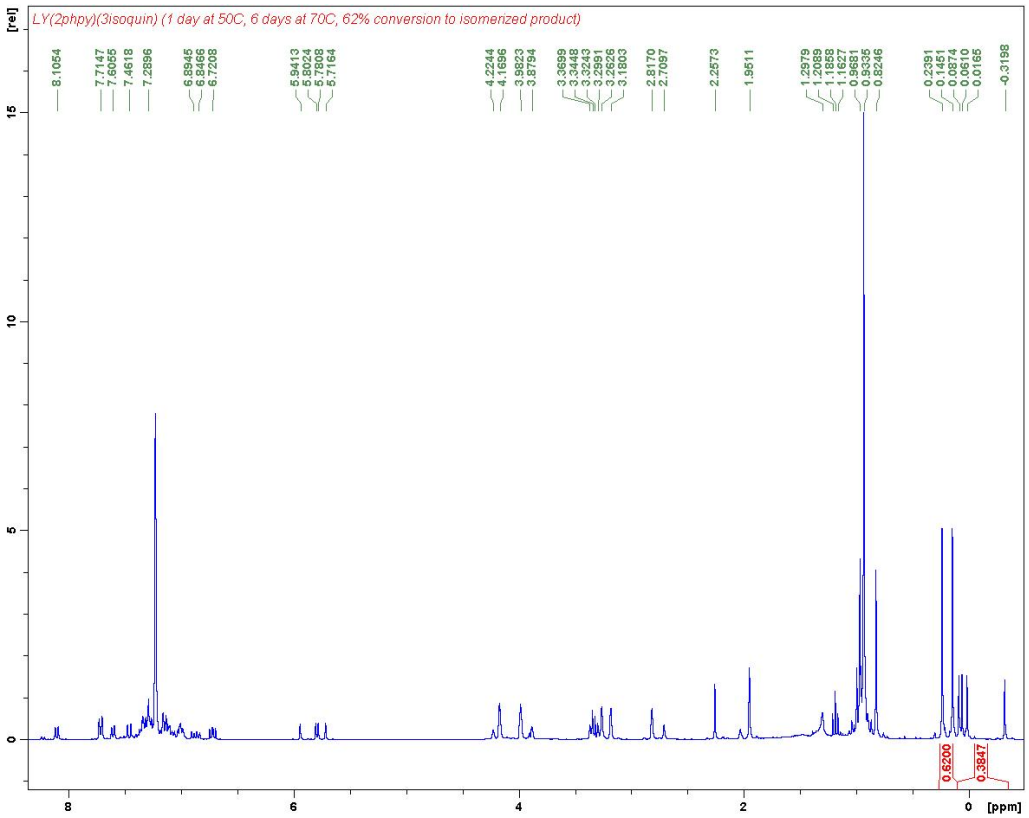
^{1}H NMR (500 MHz, C_6D_6):



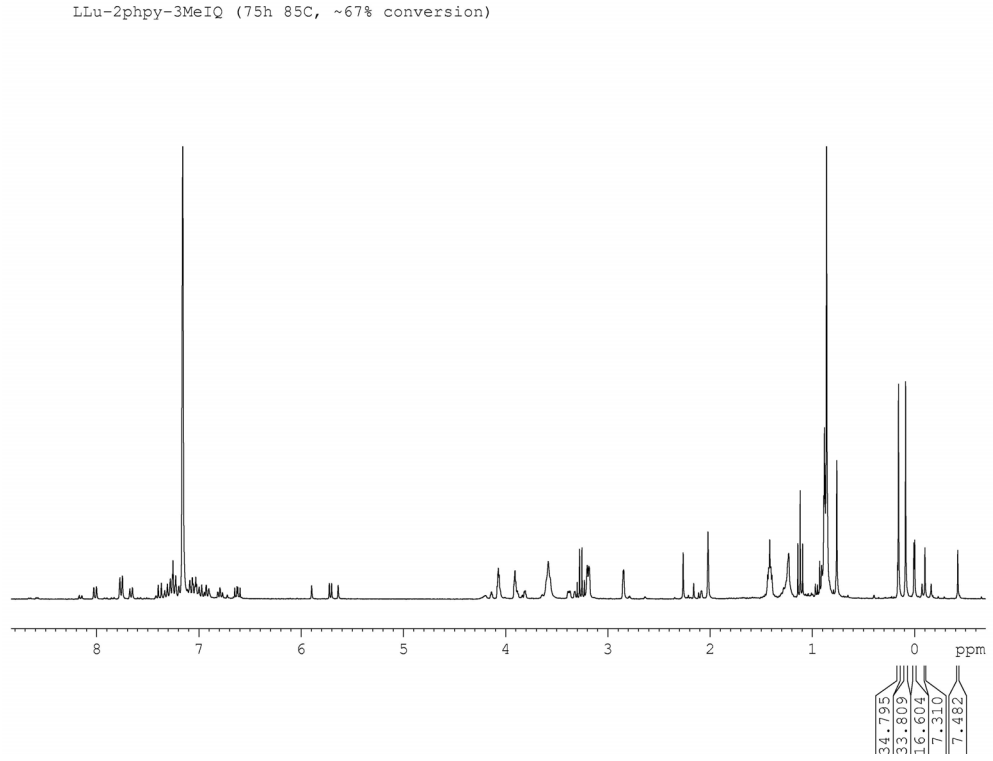
^{13}C NMR (126 MHz, C_6D_6):



7^{Y}-py^{Ph}-iqn

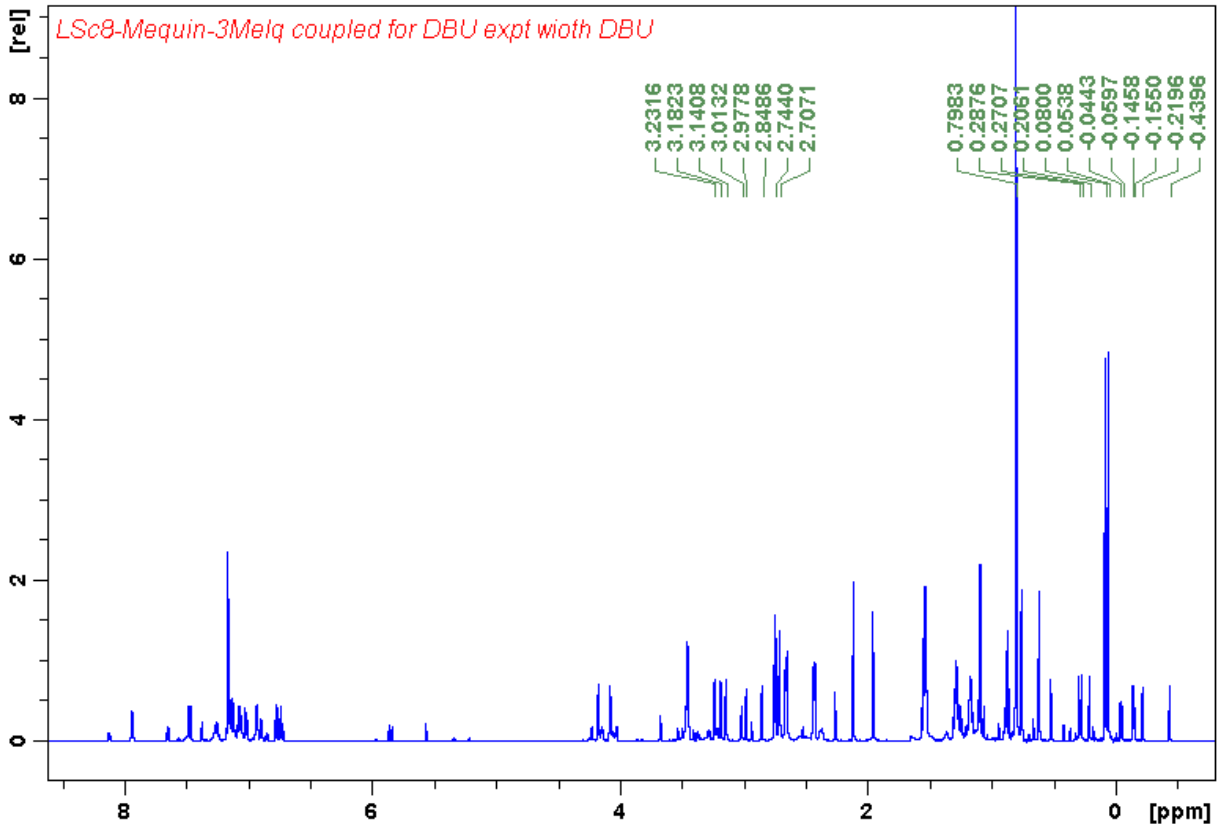


7^{Lu}-py^{Ph}-iqn

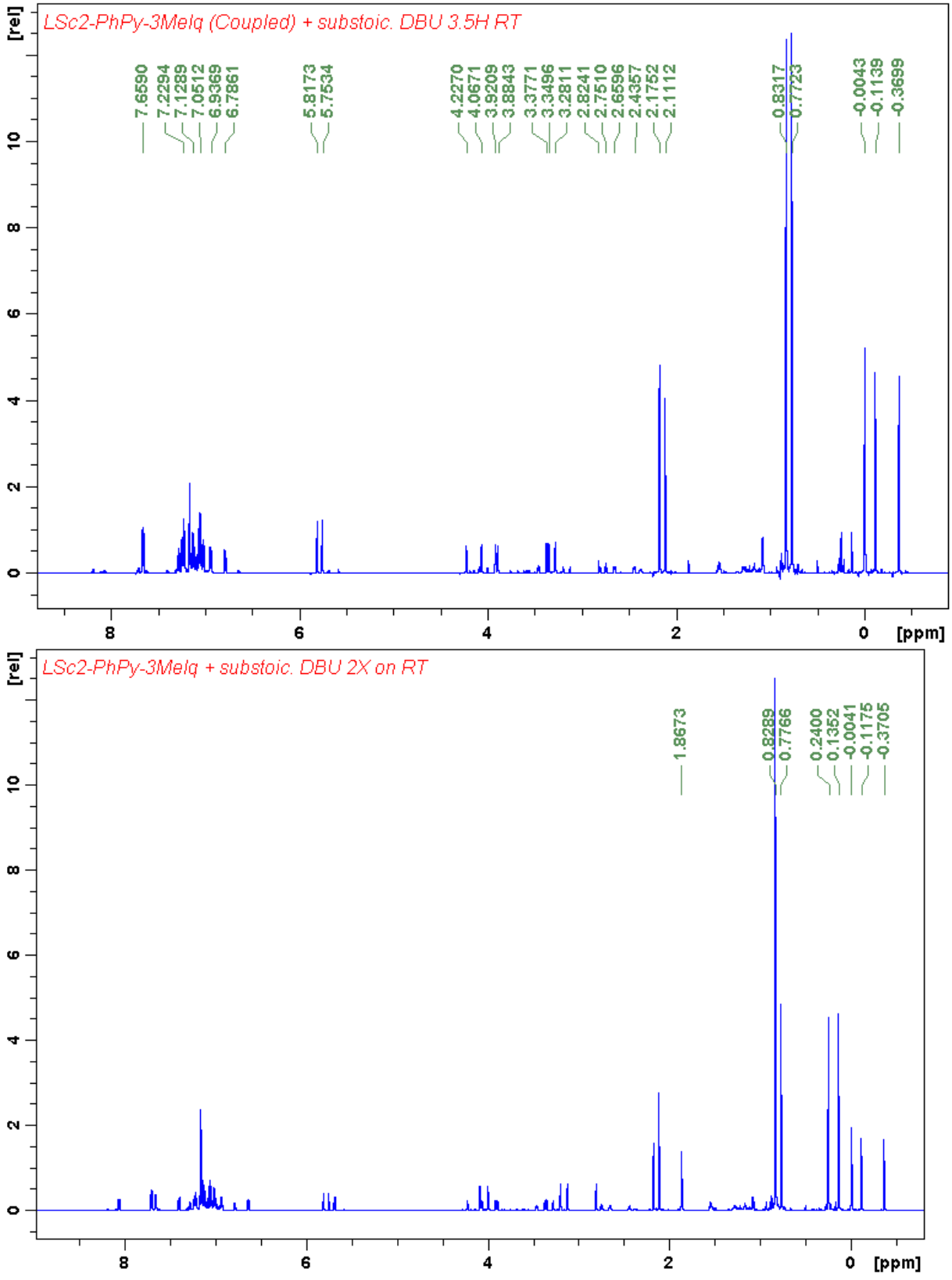


DBU-mediated reactions:

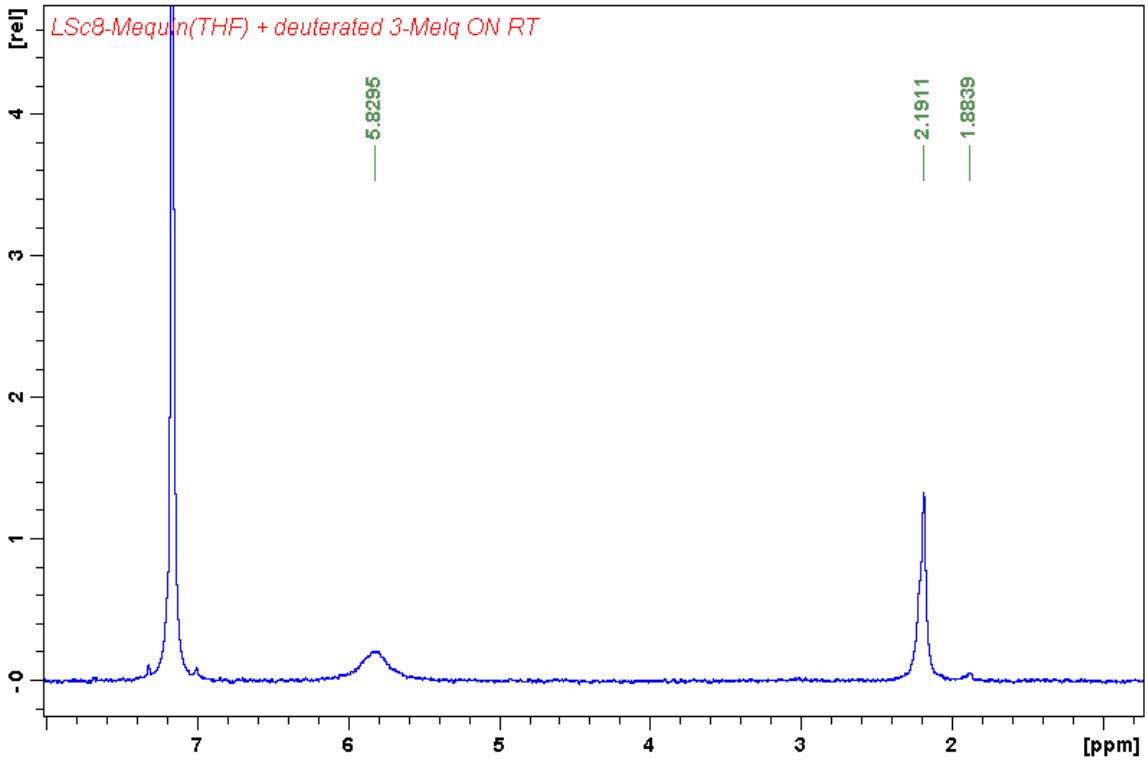
6^{Sc}-qn-iqn

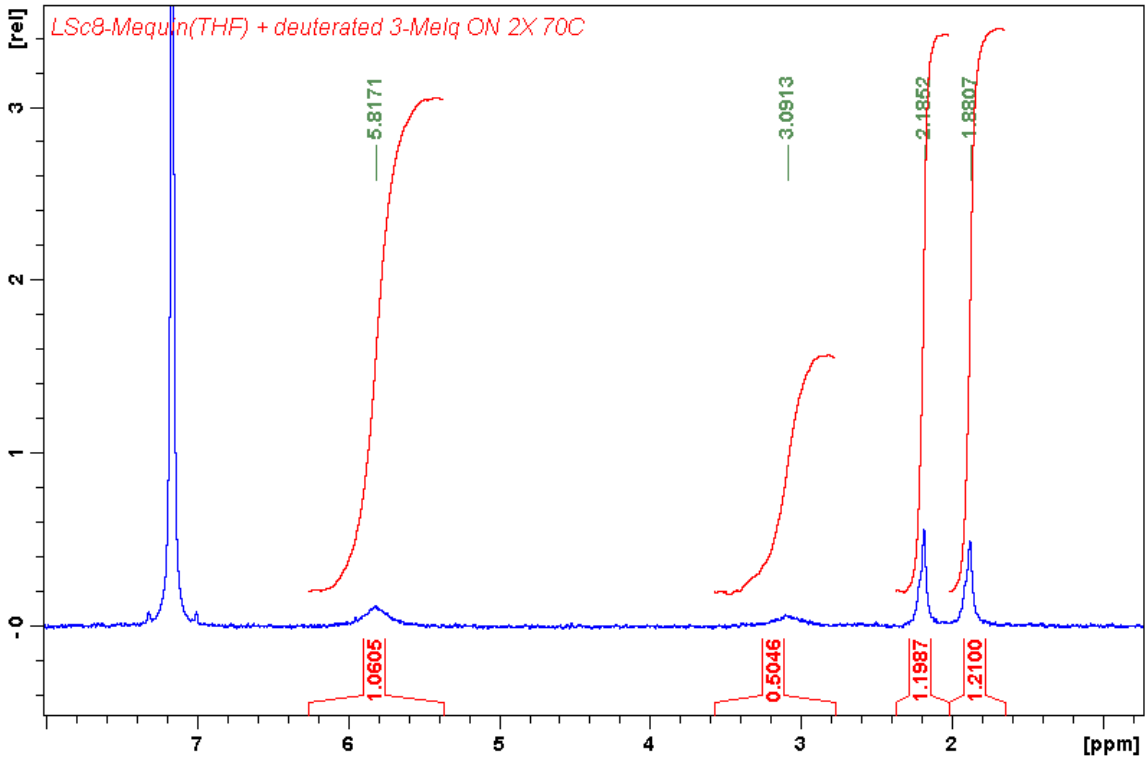


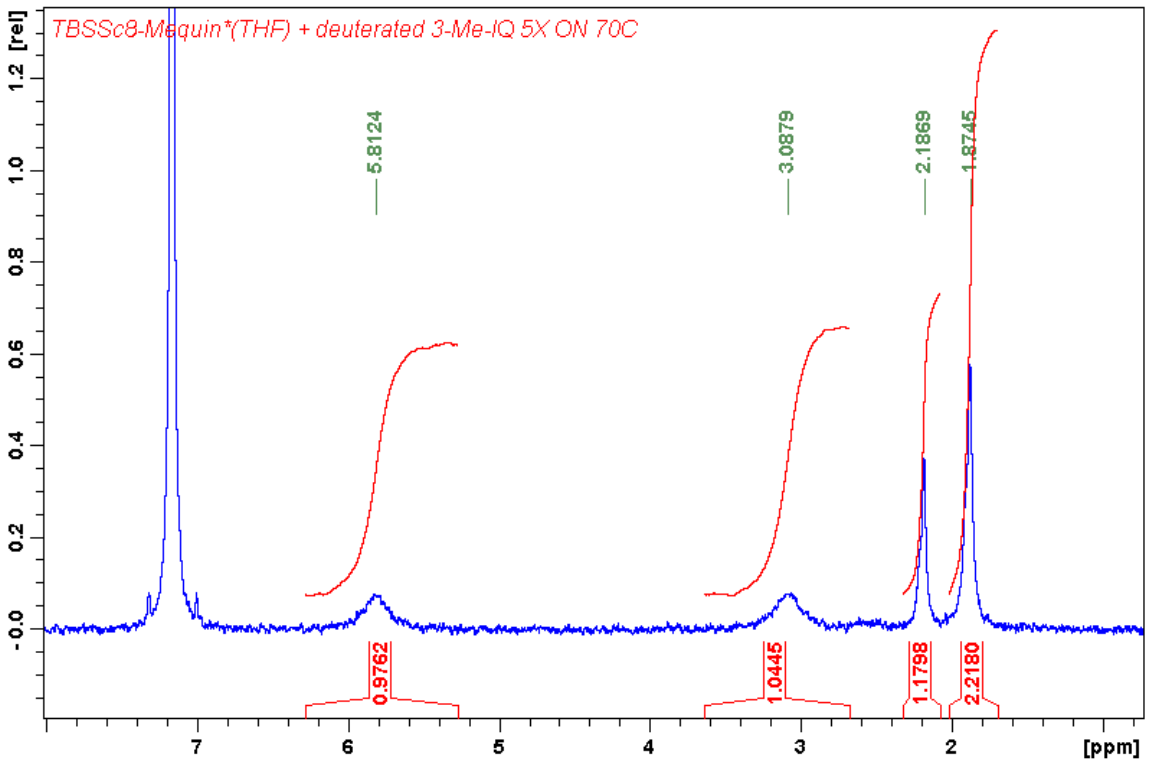
6^{Sc}-py^{Ph}-iqn

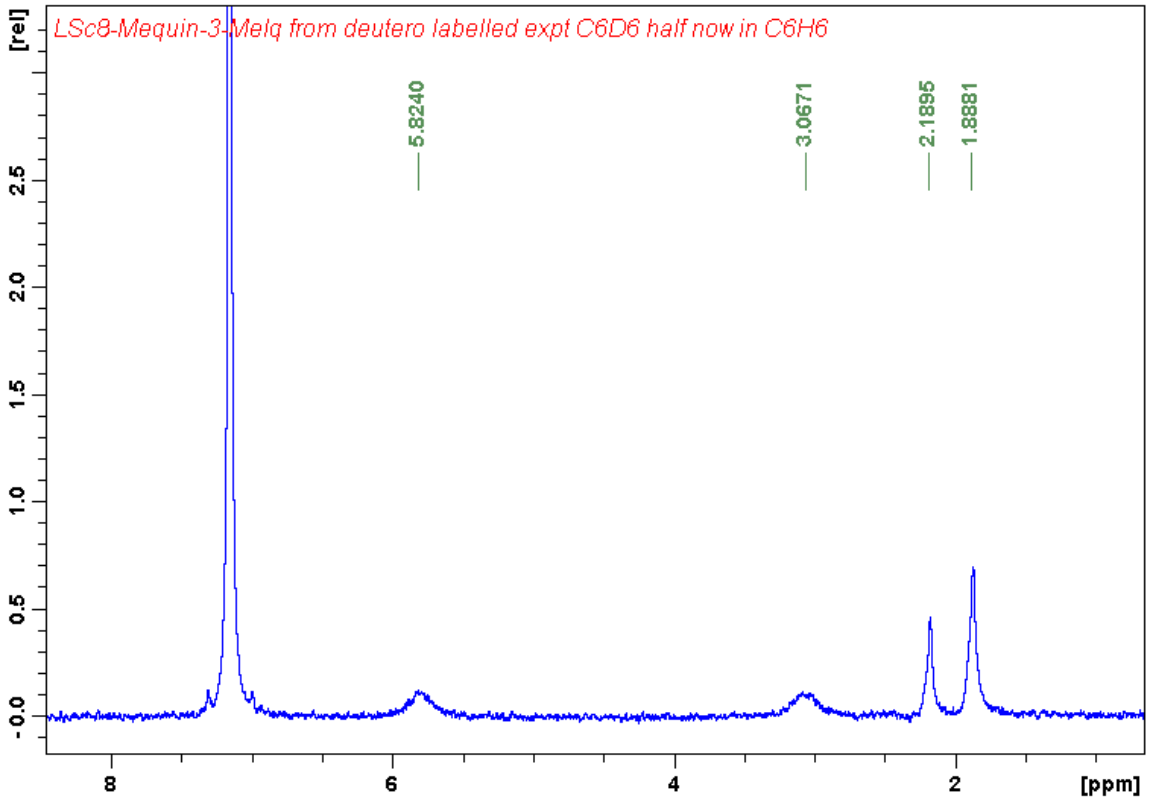

LSc2-PhPy-3Melq (Coupled) + substoic. DBU 3.5H RT
[rel]
7.6590
7.2294
7.1289
7.0512
6.9369
6.7861
5.8173
5.7534
4.2270
4.0671
3.9209
3.8843
3.3771
3.3496
3.2811
2.8241
2.7510
2.6596
2.4357
2.1752
2.1112
0.8317
0.7723
-0.0043
-0.1139
-0.3699
[ppm]
LSc2-PhPy-3Melq + substoic. DBU 2X on RT
[rel]
1.8673
0.8289
0.7766
0.2400
0.1352
-0.0041
-0.1175
-0.3705
[ppm]

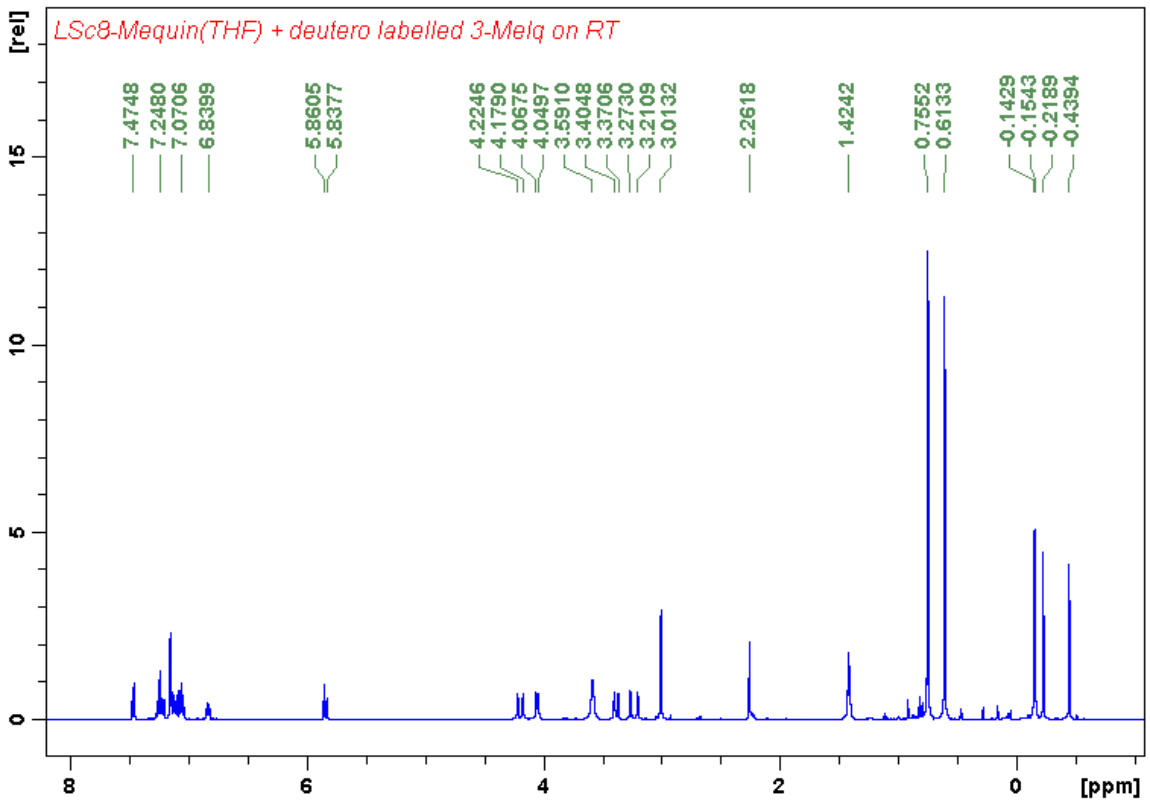
Deuterium labeling experiment:

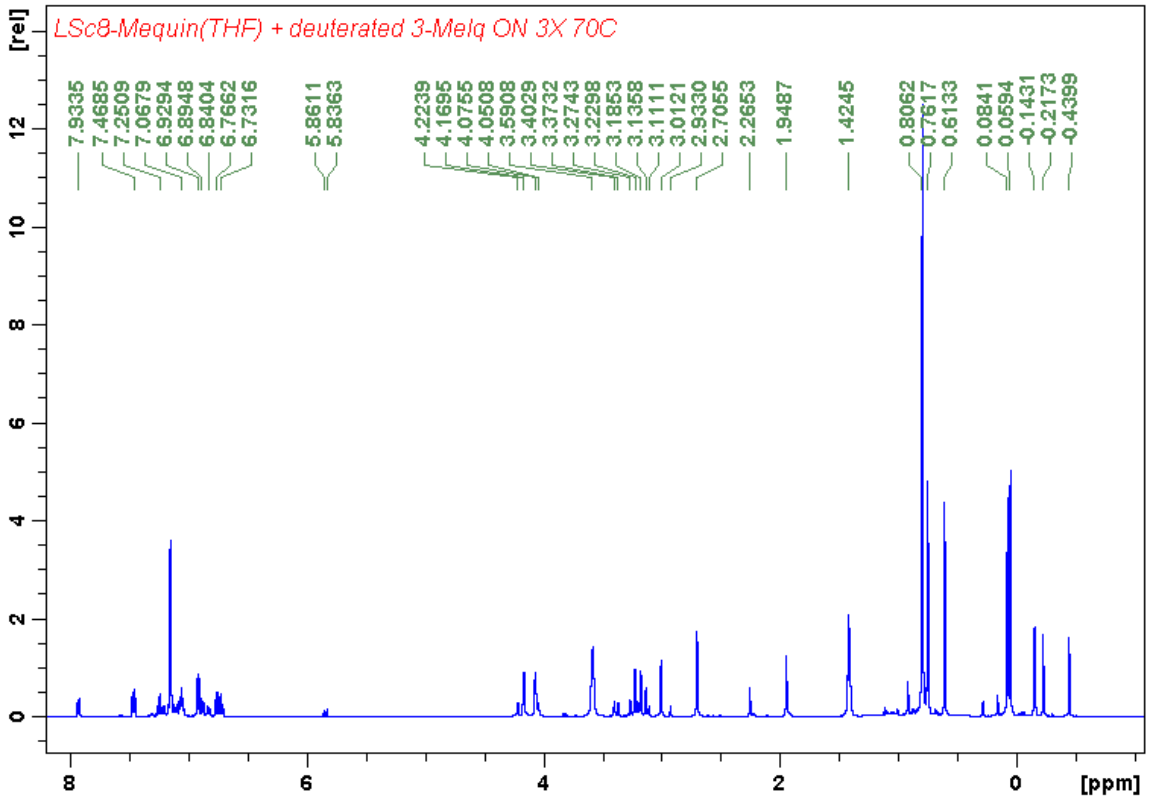


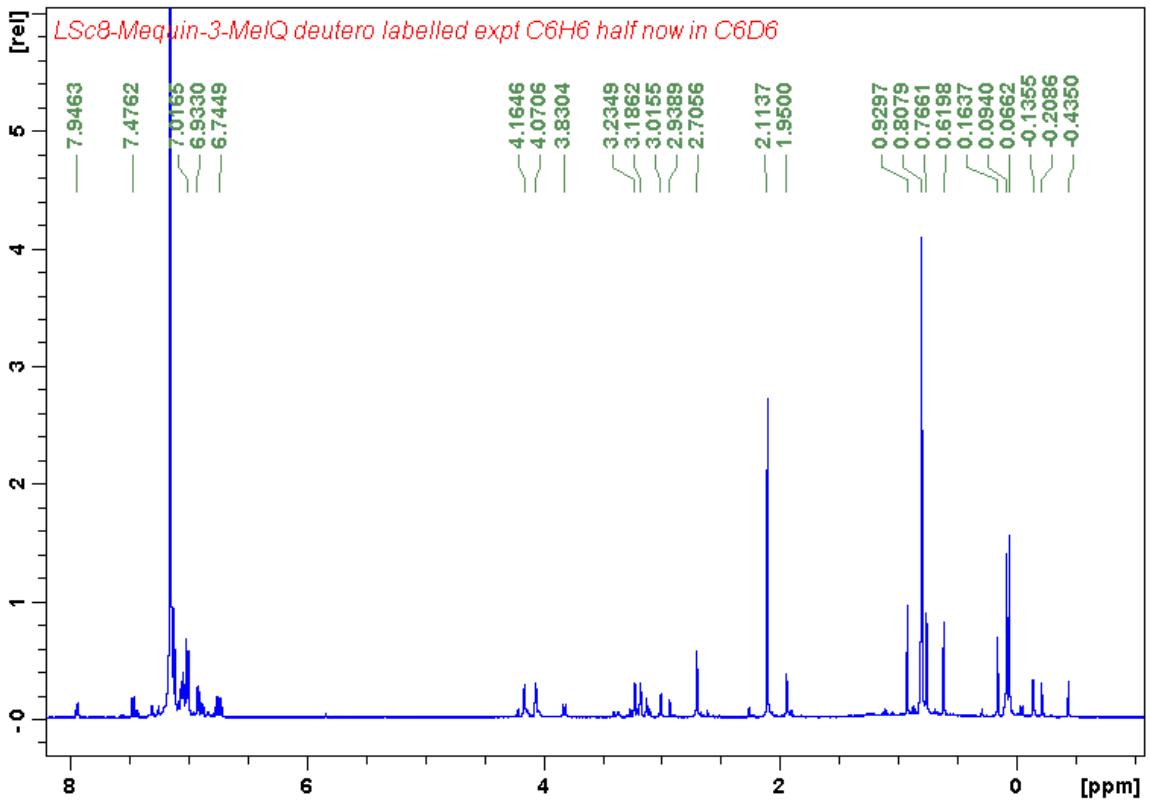



TBSSc8-Mequin*(THF) + deuterated 3-Me-IQ 5X ON 70C
5.8124
3.0879
2.1869
1.8745
0.9762
1.0445
1.1798
2.2180
[rel]
[ppm]

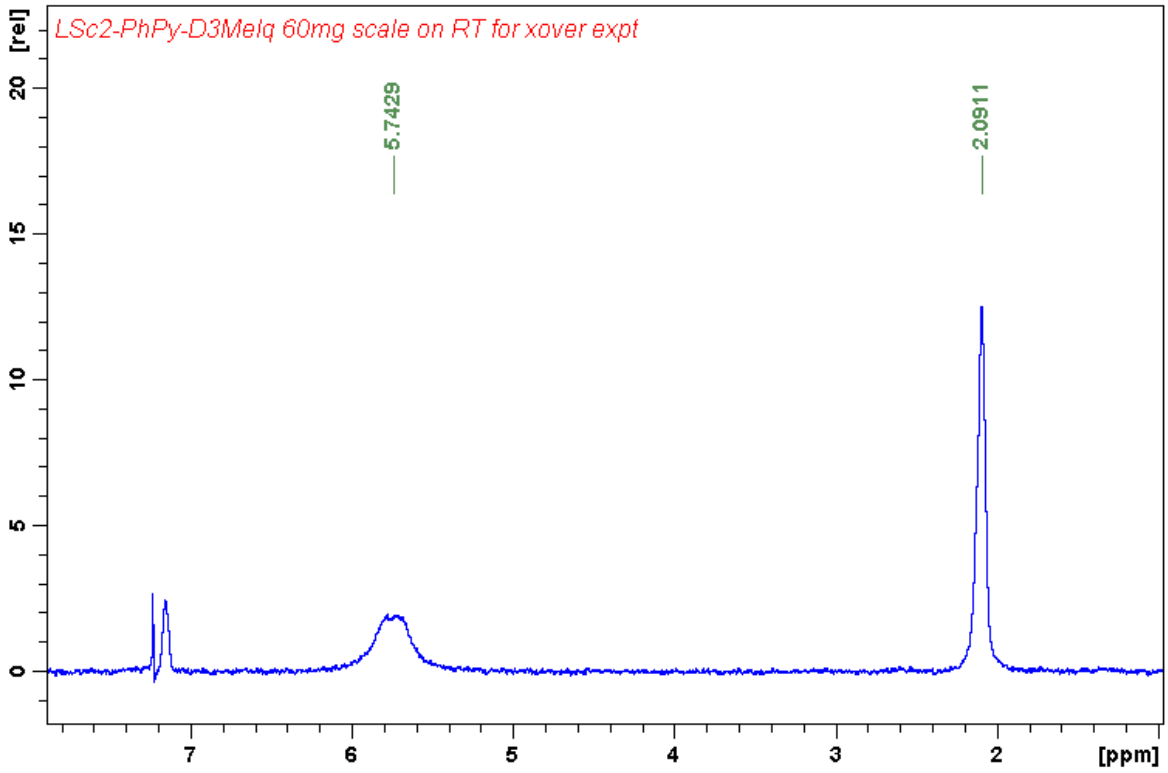

LSc8-Mequin-3-MeIq from deutero labelled expt C6D6 half now in C6H6
5.8240
3.0671
2.1895
1.8881
[rel]
[ppm]

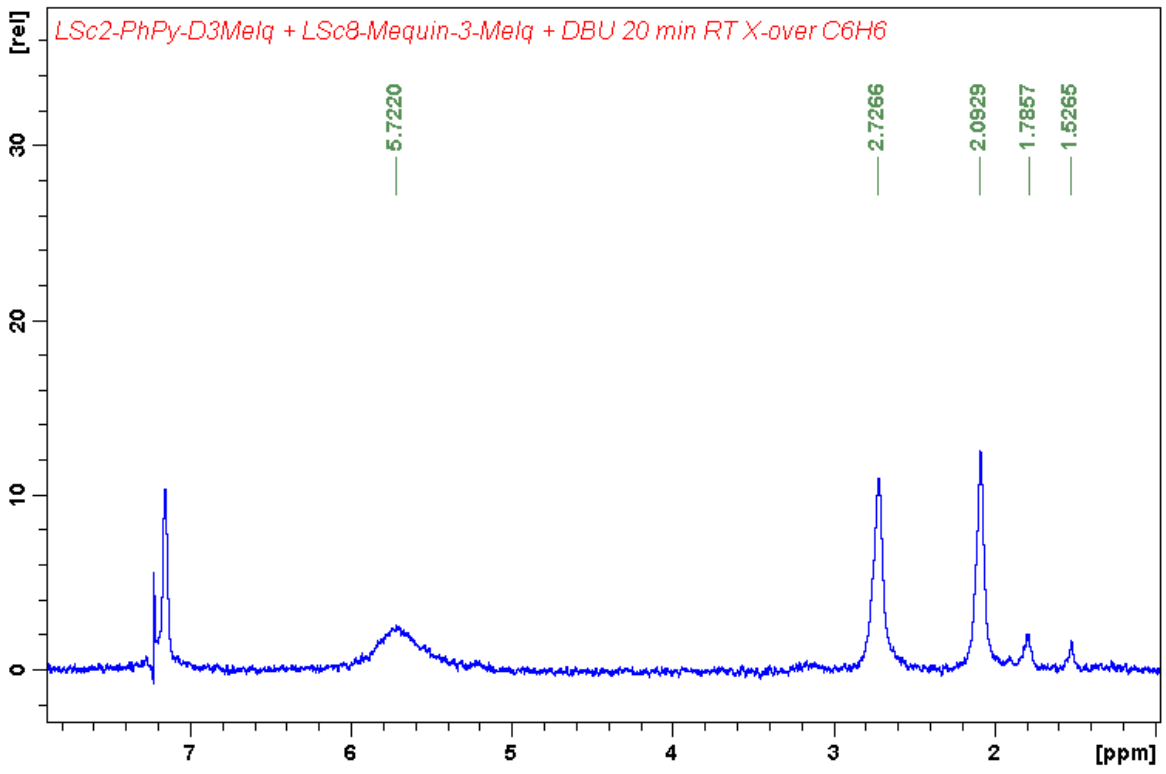

LSc8-Mequin(THF) + deutero labelled 3-Melq on RT
[rel]
7.4748
7.2480
7.0706
6.8399
5.8605
5.8377
4.2246
4.1790
4.0675
4.0497
3.5910
3.4048
3.3706
3.2730
3.2109
3.0132
2.2618
1.4242
0.7552
0.6133
-0.1429
-0.1543
-0.2189
-0.4394
[ppm]

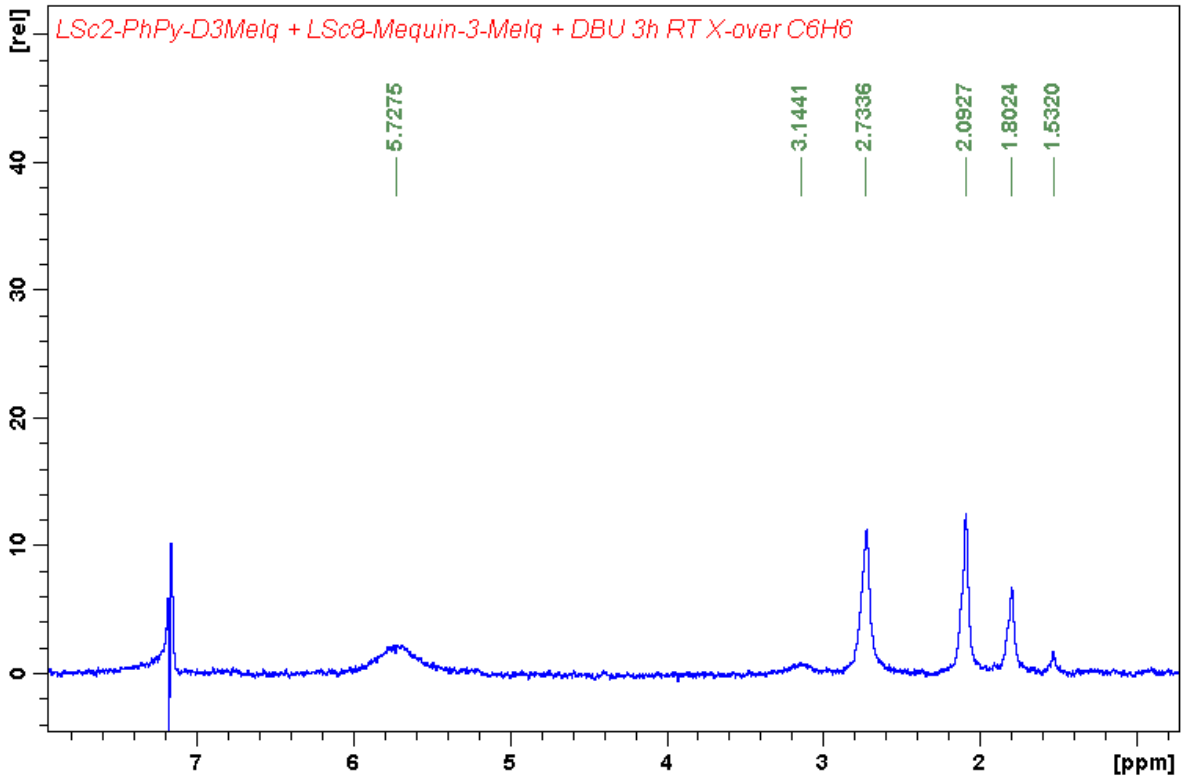

LSc8-Mequin(THF) + deuterated 3-Melq ON 3X 70C
[rel]
7.9335
7.4685
7.2509
7.0679
6.9294
6.8948
6.8404
6.7662
6.7316
5.8611
5.8363
4.2239
4.1695
4.0755
4.0508
3.5908
3.4029
3.3732
3.2743
3.2298
3.1853
3.1358
3.1111
3.0121
2.9330
2.7055
2.2653
1.9487
1.4245
0.8062
0.7617
0.6133
0.0841
0.0594
-0.1431
-0.2173
-0.4399
[ppm]



Attempted cross-over experiment in the presence of DBU:




LSc2-PhPy-D3Melq + LSc8-Mequin-3-Melq + DBU 20 min RT X-over C6H6
[rel]
5.7220
2.7266
2.0929
1.7857
1.5265
[ppm]


LSc2-PhPy-D3Melq + LSc8-Mequin-3-Melq + DBU 3h RT X-over C6H6
[rel]
5.7275
3.1441
2.7336
2.0927
1.8024
1.5320
[ppm]

X-ray crystal structures. X-ray quality crystals were obtained from various concentrated solutions placed in a -35 °C freezer in the glove box. Inside the glove box, the crystals were coated with oil (STP Oil Treatment) on a microscope slide, which was brought outside the glove box. The X-ray data collections were carried out on a Bruker AXS single crystal X-ray diffractometer using Mo$K_\alpha$radiation and a SMART APEX CCD detector. The data was reduced by SAINTPLUS and an empirical absorption correction was applied using the package SADABS. The structures were solved and refined using SHELXTL (Brucker 1998, SMART, SAINT, XPREP AND SHELXTL, Brucker AXS Inc., Madison, Wisconsin, USA). All atoms were refined anisotropically and hydrogen atoms were placed in calculated positions unless specified otherwise. Tables with atomic coordinates and equivalent isotropic displacement parameters, with all the bond lengths and angles, and with anisotropic displacement parameters are listed in the cif files.

1^{Lu}-THF. X-ray quality crystals were obtained from a concentrated Et_2O solution placed in a -35 °C freezer in the glove box. A total of 10611 reflections ($-15 \le h \le 15$, $-24 \le k \le 24$, $-26 \le l \le 26$) were collected at $T = 100(2)$ K with $2\theta_{max} = 60.96°$, of which 8733 were unique ($R_{int} = 0.0363$). The residual peak and hole electron density were 0.91 and -0.50 eA^{-3}. The least-squares refinement converged normally with residuals of $R_1 = 0.0269$ and GOF = 1.031. Crystal and refinement data for **1^{Lu}-THF**: formula $C_{35}H_{57}N_2Si_2FeLu$, space group $P2(1)/c$, $a = 11.249(2)$, $b = 17.344(3)$, $c = 18.910(4)$, $\beta = 97.509(2)°$, $V = 3657.6(12)$ Å^3, $Z = 4$, $\mu = 3.174$ mm^{-1}, F(000) = 1656, $R_1 = 0.0372$ and $wR_2 = 0.0577$ (based on all 10611 data, $I > 2\sigma(I)$).

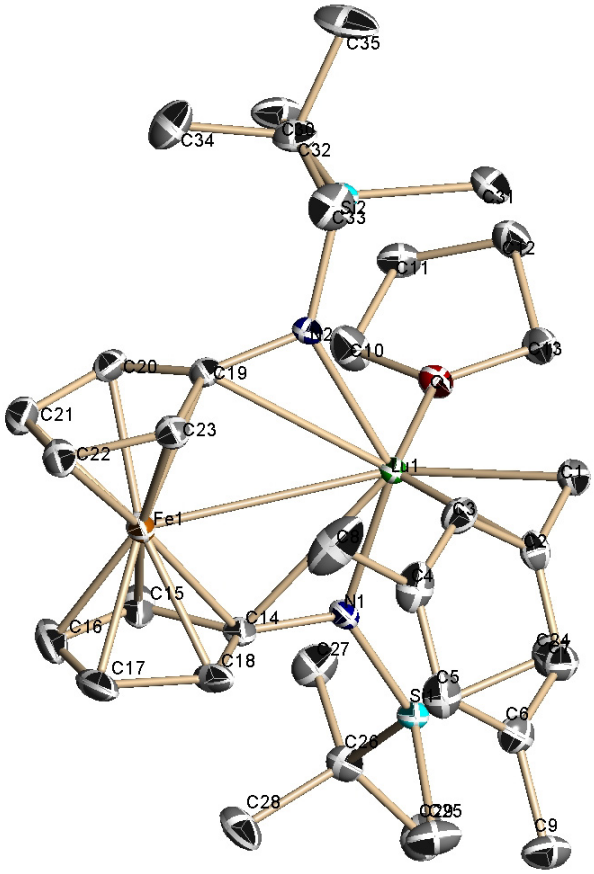


Figure SX1. Thermal ellipsoid (50% probability) representation of **1^{Lu}-THF**. Hydrogen atoms were omitted for clarity.

6^{Sc}-py^{Ph}-iqn

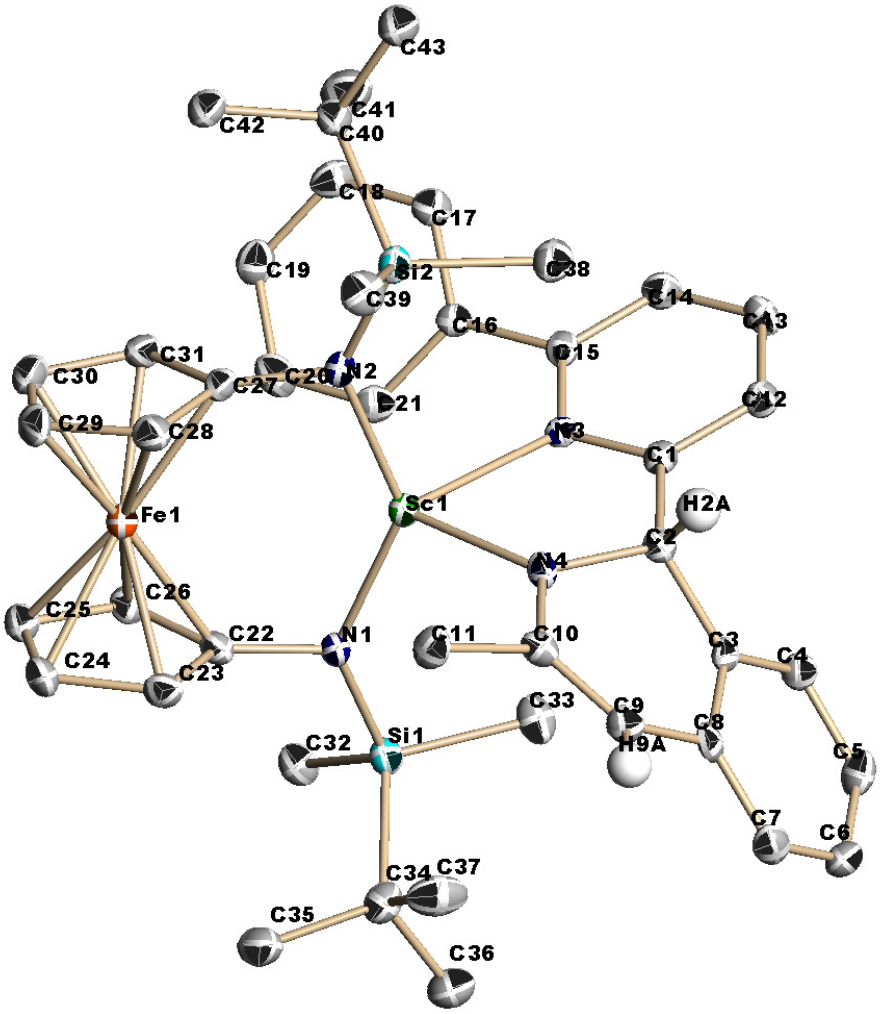


Figure SX2. Thermal ellipsoid (50% probability) representation of **6^{Sc}-py^{Ph}-iqn**. Irrelevant hydrogen atoms were omitted for clarity.

7^{Sc}-py^{Ph}-iqn

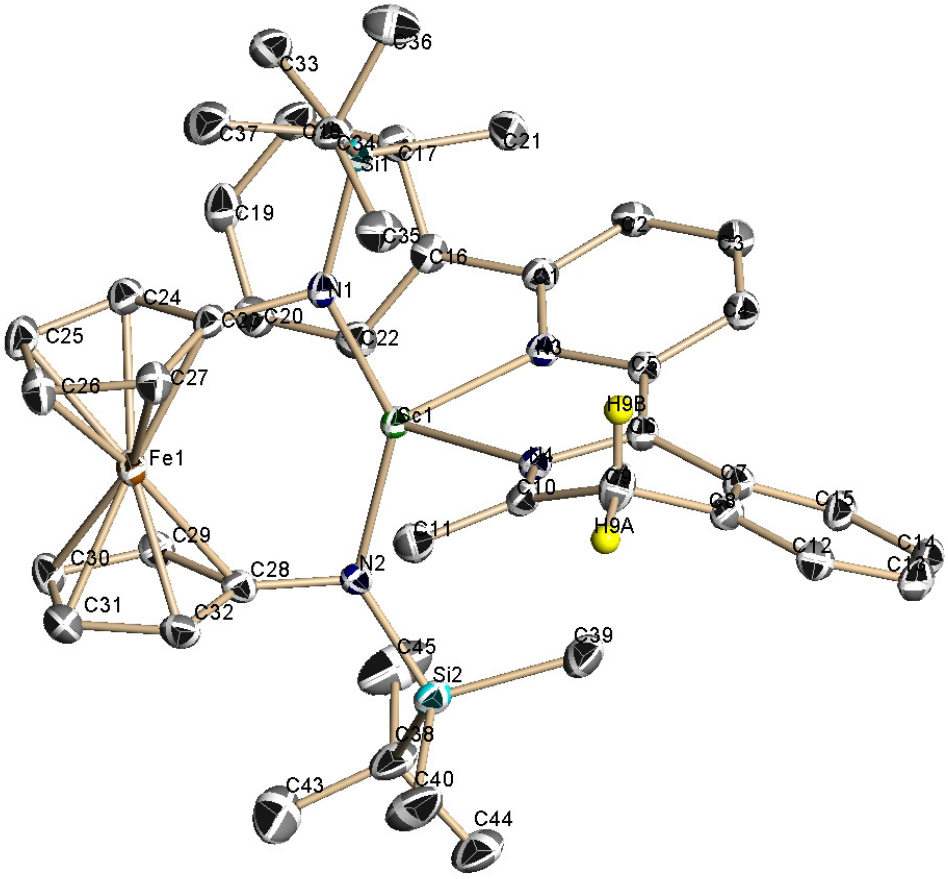


Figure SX3. Thermal ellipsoid (50% probability) representation of **7^{Sc}-py^{Ph}-iqn**. Irrelevant hydrogen atoms were omitted for clarity.

X-ray crystal structure of 7^{Sc}-qn-iqn. X-ray quality crystals were obtained from a concentrated Et_2O : pentane solution placed in a -35 °C freezer in the glove box. The data collected were of not very good quality and some of the atoms were disordered. Both silyl groups were disordered, one in 75/25 % and the other 90/10 %. Both disorders were modeled. Some of the disordered counterparts (Si2A, C32A – C34A, C36A, C37A – C42A) were refined only isotropically. A total of 8153 reflections ($-14 \le h \le 14$, $-41 \le k \le 41$, $-13 \le l \le 13$) were collected at T = 100(2) K with $2\theta_{max}$ = 52.86°, of which 4153 were unique (R_{int} = 0.1188). The residual peak and hole electron density were 1.65 and -0.69 eA^{-3}. The least-squares refinement converged normally with residuals of R_1 = 0.0843 and GOF = 1.036. Crystal and refinement data for **7^{Sc}-qn-iqn**: formula $C_{42}H_{49}N_4Si_2FeSc$, space group $P2(1)/c$, a = 11.5417(17), b = 33.162(5), c = 11.1501(17), β = 110.935(2)°, V = 3985.9(10) Å^3, Z = 4, μ = 0.628 mm^{-1}, F(000) = 1640, R_1 = 0.1532 and wR_2 = 0.2331 (based on all 8153 data, $I > 2\sigma(I)$).

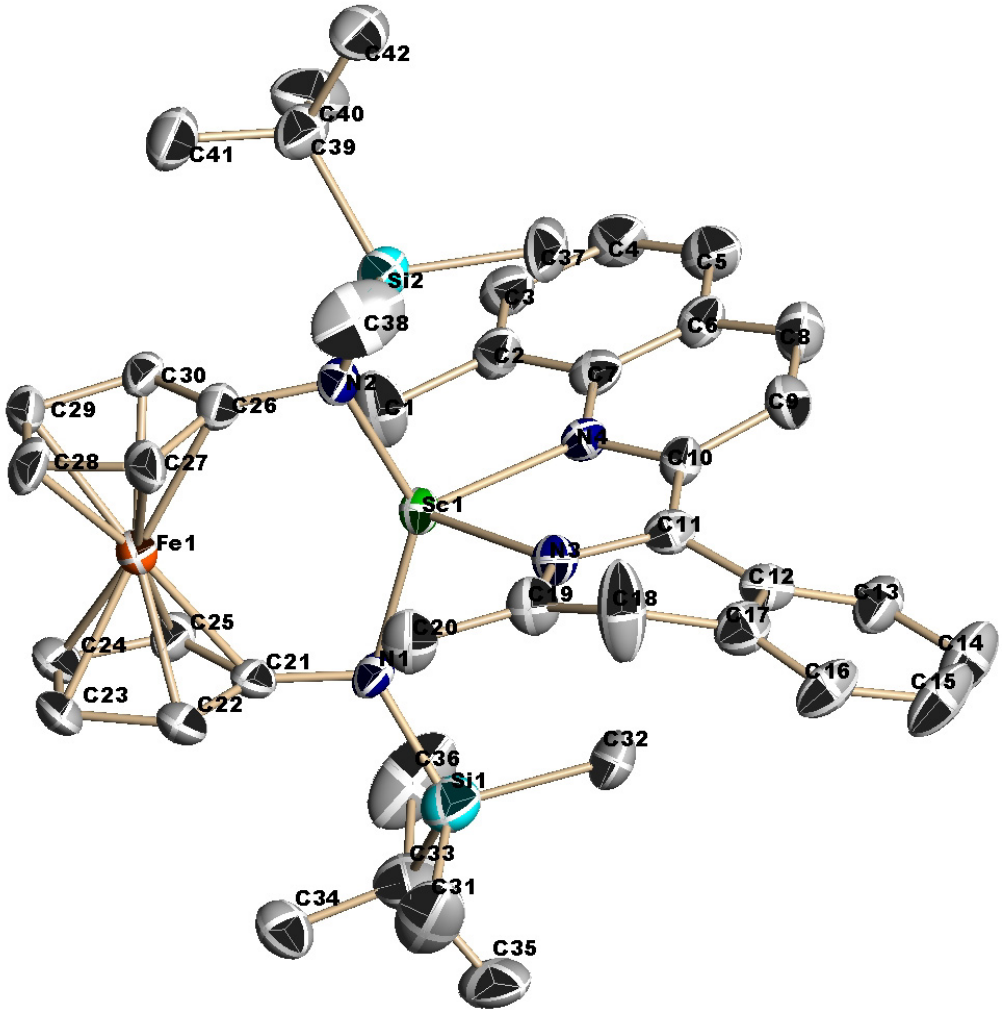


Figure SX4. Thermal ellipsoid (50% probability) representation of **7^{Sc}-qn-iqn**. Hydrogen atoms and disordered counterparts were omitted for clarity.

Computational details

Comparison of metrical parameters

Complex	Parameter	Jaguar	ADF	Experimental
6^{Sc}-py^{Ph}-iqn	Sc-N1	2.33 Å	2.37 Å	2.30 Å
	Sc-N2	2.09 Å	2.14 Å	2.09 Å
	N1-C1	1.35 Å	1.36 Å	1.36 Å
	C1-C2	1.51 Å	1.51 Å	1.50 Å
	N2-C2	1.46 Å	1.47 Å	1.47 Å
	N2-C3	1.38 Å	1.38 Å	1.38 Å
	C3-C4	1.37 Å	1.38 Å	1.37 Å
	$Sc\text{-}N_{amide}$	2.06 Å	2.10 Å	2.05 Å
	$Sc\text{-}N_{amide}$	2.07 Å	2.11 Å	2.07 Å
	N1ScN2	76.2°	75.0°	73.7
	ScN1C1	111.0°	112.7°	113.0°
	N1C1C2	119.1°	119.4°	118.6°
	N2C2C1	111.7°	112.0°	110.7°
	ScN2C2	119.9°	120.1°	120.5°
	$N_{amide}ScN_{amide}$	133.2°	136.5°	135.9°
7^{Sc}-py^{Ph}-iqn	Sc-N1	2.19 Å	2.24 Å	2.18 Å
	Sc-N2	2.22 Å	2.27 Å	2.22 Å
	N1-C1	1.39 Å	1.41 Å	1.39 Å
	C1-C2	1.41 Å	1.42 Å	1.40 Å
	N2-C2	1.41 Å	1.41 Å	1.41 Å
	N2-C3	1.31 Å	1.31 Å	1.31 Å
	C3-C4	1.50 Å	1.51 Å	1.48 Å
	$Sc\text{-}N_{amide}$	2.05 Å	2.08 Å	2.04 Å
	$Sc\text{-}N_{amide}$	2.06 Å	2.10 Å	2.06 Å
	N1ScN2	76.4°	74.7°	75.0°
	ScN1C1	113.5°	114.5°	115.8°
	N1C1C2	119.2°	118.9°	118.2°
	N2C2C1	116.6°	116.8°	116.0°
	ScN2C2	113.0°	114.8°	114.5°
	$N_{amide}ScN_{amide}$	132.9°	138.7°	140.4°

Details for calculations carried out with Jaguar

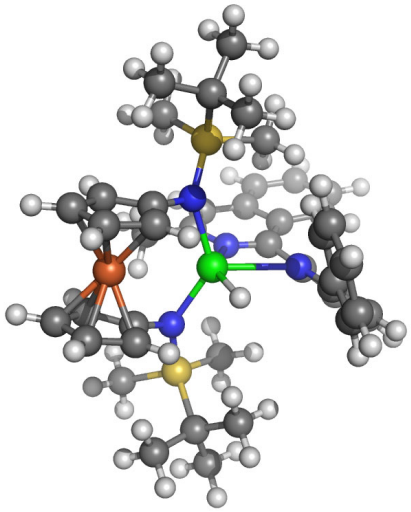


Figure SX5. Structure for $\mathbf{I_H}^{6\text{-}7}$ (B3LYP/LACVP**). The H atom is placed away from the isoquinoline heterocycle. The angle of the pyridyl ligand is distorted from the planar conformation that is necessary for the best orbital overlap.

6^{Sc}-py^{Ph}-iqn

Fe1	0.6048098450	1.0644467739	8.8310073419
Sc2	3.2102251720	2.3257423193	10.6207437116
Si3	2.9908447270	5.1689477944	8.5100904086
Si4	2.8633133674	-0.4670021125	12.7585080595
N5	2.4162758231	0.5993476149	11.4274001811
N6	2.6863739928	3.5045574828	9.0063133449
N7	5.5410783920	2.3836089733	10.5631989195
N8	3.7165033672	3.5861760216	12.2023965128
C9	5.8635277783	0.7537125084	8.7532711043
C10	7.6586711971	2.3347597181	9.4254491684
H11	8.2832278000	1.8883426248	8.6603142806
C12	1.2940998327	-0.7487188338	9.5720765534
H13	2.1660067379	-1.2626789696	9.1968689497
C14	2.8644492275	4.1403087355	13.1383328326
C15	4.5947759031	4.0613169665	14.8529102869
C16	6.3545151315	1.8682301080	9.6013716337
C17	1.3088246621	0.2164752504	10.6432715314
C18	6.0228565079	3.3396644842	11.3896636859
C19	3.0729798587	-2.2537296151	12.1292571177
H20	3.9384443429	-2.3382923955	11.4611960882
H21	2.1940128115	-2.6071346761	11.5810975867
H22	3.2431386528	-2.9451203375	12.9631188214
C23	8.1451069415	3.3418318420	10.2552891801
H24	9.1557109052	3.7195892237	10.1289946971
C25	4.9279262672	3.9743396395	16.2159001036
H26	4.2109610971	4.3196251181	16.9572940744
C27	1.5730287501	-0.5062889778	14.2056947769
C28	6.1237671797	0.7497751681	7.3720643363
H29	6.5933028306	1.6146535978	6.9123768494
C30	6.1461444117	3.4346884224	16.6187153288

H31	6.3876937872	3.3772049076	17.6770713603
C32	6.7392323561	3.0454726018	14.3089855820
H33	7.4533934208	2.6782114705	13.5776007863
C34	4.5363039255	0.0886908604	13.4424446353
H35	5.2881482394	0.1930913287	12.6520842965
H36	4.9161156733	-0.6552020237	14.1520081131
H37	4.4801703707	1.0475457579	13.9639608621
C38	5.1179339496	3.9164542129	12.4510198128
H39	5.2228512317	5.0173463132	12.3527808832
C40	3.6058870077	5.2985941882	6.6718952190
C41	1.4252839031	4.2942144435	12.7150950556
H42	0.8005132852	4.6433130408	13.5411867586
H43	1.0136706887	3.3330686483	12.3780008338
H44	1.3298882953	4.9990504155	11.8808446455
C45	5.1510209178	-1.4542458574	7.1733374075
H46	4.8816441154	-2.3123156407	6.5639033453
C47	-0.0468432365	0.6959541055	10.7694725930
H48	-0.3733157928	1.4489592753	11.4731537259
C49	5.7627652875	-0.3431262968	6.5879191998
H50	5.9599930623	-0.3283758933	5.5197256940
C51	7.3216143438	3.8439608186	11.2524076274
H52	7.6578752250	4.6260502349	11.9231751843
C53	4.8902517899	-1.4596003724	8.5435706218
H54	4.4269047927	-2.3253288362	9.0081070081
C55	7.0500256857	2.9545263319	15.6688956181
H56	7.9960064796	2.5203955808	15.9804129429
C57	0.3295673248	-1.3394936496	13.8237778618
H58	-0.3920867519	-1.3482182123	14.6539729335
H59	0.5864334263	-2.3831230889	13.6092548202
H60	-0.1860240428	-0.9374555912	12.9459135804
C61	3.2932684501	4.4990201080	14.3869022603
H62	2.5948362441	4.9326120426	15.0950178037
C63	5.5354012756	3.6119381400	13.8938055445
C64	4.1209559003	6.7312161441	6.4039513061
H65	4.4380674627	6.8310245597	5.3556265754
H66	4.9833942625	6.9856389340	7.0297022370
H67	3.3472223572	7.4883634538	6.5779931218
C68	5.2361709758	-0.3601872423	9.3304261495
H69	5.0490600866	-0.3796437528	10.3982435887
C70	0.6193012459	1.3827603028	6.7905193000
H71	0.4436611245	0.6025353604	6.0617846836
C72	2.4694637578	5.0031398707	5.6681578290
H73	2.8415446410	5.0917028340	4.6365503080
H74	1.6395691303	5.7111832953	5.7723583156
H75	2.0636388969	3.9942807996	5.7847625958
C76	1.8831900785	1.7512144453	7.3376342969
H77	2.8422561260	1.3171776072	7.0876590524
C78	-0.0383171659	-0.8837692804	9.0889658604
H79	-0.3592621572	-1.5183825297	8.2734833789
C80	1.4342738089	6.2492399479	8.6910969455
H81	1.0864700039	6.2537078369	9.7309816056
H82	0.6055748140	5.9018291877	8.0667496402
H83	1.6431509289	7.2894225245	8.4135274549
C84	1.6849099497	2.8150987210	8.2918438787
C85	-0.8688323510	0.0117723565	9.8282264544
H86	-1.9279001634	0.1703933728	9.6742688474

C87	4.3106132837	5.9224444030	9.6366184894
H88	3.9987407478	5.8596057591	10.6830160681
H89	4.4501688532	6.9815237235	9.3935753802
H90	5.2848101320	5.4318230051	9.5413267658
C91	4.7607423601	4.3060580554	6.4248022983
H92	5.1397168200	4.4028047858	5.3963473122
H93	4.4381878709	3.2696744635	6.5641533342
H94	5.6064632900	4.4853797508	7.1010275626
C95	-0.3820028934	2.1918204057	7.4088386395
H96	-1.4473063504	2.1277913965	7.2308589388
C97	0.2617314521	3.0502400844	8.3450569628
H98	-0.2214393268	3.7649228317	8.9961180564
C99	2.2290676741	-1.1568612768	15.4453599480
H100	1.4950033863	-1.2456875656	16.2591607173
H101	3.0669727859	-0.5632190989	15.8257091527
H102	2.6014227697	-2.1675813856	15.2378146089
C103	1.1249094279	0.9202151036	14.5825295805
H104	0.4544963481	0.8935901955	15.4545258397
H105	0.5778586656	1.3980466679	13.7640462222
H106	1.9687825333	1.5712980308	14.8378878446

7^{Sc}-py^{Ph}-iqn

Fe1	4.2452066964	8.9848765802	5.7799220272
Sc2	2.4913167052	6.3399481569	4.5407595986
Si3	4.2067605367	6.8238336486	1.5106117821
Si4	1.1098977672	5.9268901321	7.7208230668
N5	3.8615070614	7.1038727954	3.2211439119
N6	2.0088702683	6.8074209259	6.4812990294
N7	0.8117959163	5.4660981579	3.4245997409
N8	2.9075869189	4.1535118785	4.6003688526
C9	-0.1081201754	6.1577634910	2.6880996880
C10	-1.0237201815	5.5339727503	1.8600152578
H11	-1.7528845990	6.1221840695	1.3163330842
C12	-0.9942271209	4.1242145606	1.7740639079
H13	-1.6821632259	3.6058227022	1.1112779063
C14	-0.0854353476	3.4095448808	2.5080468071
H15	-0.0203214717	2.3351055312	2.4022438478
C16	0.8511742285	4.0757264859	3.3606427935
C17	1.8584454479	3.3784756043	4.0708476141
C18	1.8168713871	1.9677260390	4.4580792678
C19	3.0331295944	1.3505732851	4.8336900508
C20	4.2941186386	2.1568383198	4.6344757372
H21	5.1279895951	1.7580077352	5.2218175186
H22	4.6095966513	2.1186615016	3.5733441114
C23	4.0312462292	3.6024082631	4.9750736435
C24	5.1018317234	4.3880126645	5.6690286609
H25	4.8392826902	5.4402370518	5.8035489506
H26	6.0457903730	4.3385896411	5.1099101199
H27	5.2999167165	3.9666124011	6.6639070714
C28	3.0483358662	0.0614991546	5.3647028875
H29	3.9988755938	-0.3811400585	5.6557801213
C30	1.8660207781	-0.6631848069	5.5070061325
H31	1.8863203455	-1.6734313740	5.9056634233
C32	0.6550814068	-0.0667203057	5.1451655005
H33	-0.2788352693	-0.6069214897	5.2783687515
C34	0.6258359651	1.2310394828	4.6470530432
H35	-0.3331526978	1.6953939755	4.4444177783

C36	-0.1358630918	7.6413321197	2.8097561742
C37	-0.1814508014	8.4367310404	1.6518650919
H38	-0.1206192152	7.9589481631	0.6783456388
C39	-0.2937696844	9.8222132988	1.7432229695
H40	-0.3182475679	10.4221647903	0.8375195892
C41	-0.3774480271	10.4381232226	2.9943130873
H42	-0.4792218471	11.5175855559	3.0665031975
C43	-0.3400166878	9.6580378176	4.1497279462
H44	-0.4343510579	10.1280165836	5.1248752380
C45	3.1776079979	5.3452607466	0.9305549257
H46	2.1062676862	5.5605707213	0.9787931547
H47	3.3585360502	4.4441212120	1.5261046465
H48	3.4146245634	5.1073814149	-0.1122166221
C49	-0.2118598615	8.2692835061	4.0626363602
H50	-0.2157514709	7.6727204288	4.9702570500
C51	4.5120894469	8.1945435958	3.8340147684
C52	4.1051096645	9.5771318056	3.7869981634
H53	3.2021063993	9.9347226215	3.3113193970
C54	5.0710763619	10.3653749257	4.4745893163
H55	5.0275519583	11.4356404613	4.6274963284
C56	6.0799130672	9.4895898548	4.9785247128
H57	6.9337066877	9.7814803942	5.5756483861
C58	5.7325534603	8.1589221987	4.6046740533
H59	6.2879253114	7.2642524457	4.8454832709
C60	2.7803767636	7.9172945280	6.8762053432
C61	2.4324843378	9.3094498886	6.7218166219
H62	1.5504514060	9.6724765819	6.2175903867
C63	3.4493678839	10.1099137828	7.3169793997
H64	3.4765730632	11.1912875963	7.3415599219
C65	4.4566903623	9.2351984294	7.8250455124
H66	5.3790498087	9.5391756616	8.3020138393
C67	4.0597405123	7.8965990883	7.5436989469
H68	4.6134340140	7.0012058188	7.7888607361
C69	3.7055007216	8.3464257414	0.4915627332
H70	2.6355884254	8.5488758141	0.6105217914
H71	3.9024394728	8.2024810691	-0.5775108817
H72	4.2474851634	9.2431982420	0.8093791550
C73	6.0814492431	6.4579637666	1.1483950489
C74	6.6260703162	5.3793532328	2.1065768120
H75	7.6706768553	5.1365202683	1.8625613042
H76	6.0516437576	4.4468665838	2.0430667208
H77	6.6003029425	5.7142760661	3.1476932213
C78	6.2247315987	5.9375274627	-0.3009294133
H79	7.2865144323	5.7863071532	-0.5435991189
H80	5.8254664348	6.6450950155	-1.0373815673
H81	5.7183637785	4.9779566320	-0.4492850181
C82	6.9473284713	7.7315058603	1.2772701787
H83	7.9995036190	7.4977283307	1.0570944111
H84	6.9110137982	8.1631150181	2.2811608017
H85	6.6355908432	8.5080472729	0.5698159424
C86	0.1218661662	7.0830023152	8.9300943146
C87	-0.1150986111	4.7858955516	6.8414706858
H88	0.3923258286	4.1145613536	6.1424798455
H89	-0.8728612738	5.3416028570	6.2783078835
H90	-0.6380702304	4.1573129471	7.5706121487
C91	2.2957324312	4.8527075472	8.7456185110

H92	2.7970019775	4.1286420481	8.0930479882
H93	1.7715375826	4.2868148891	9.5245030134
H94	3.0694546271	5.4528532928	9.2367299269
C95	1.0583451629	7.8790979370	9.8662531324
H96	0.4659589285	8.4933499178	10.5606120447
H97	1.7215343580	8.5534418389	9.3178117788
H98	1.6837400144	7.2171412235	10.4760593067
C99	-0.7970938767	6.2040038431	9.8108755624
H100	-1.3416670856	6.8316961296	10.5311342827
H101	-0.2320931045	5.4653855178	10.3915001459
H102	-1.5452590348	5.6644709896	9.2202187497
C103	-0.7635903565	8.0737096127	8.1453010657
H104	-1.3684851081	8.6796083350	8.8358478536
H105	-1.4610503704	7.5599146717	7.4726139430
H106	-0.1631045171	8.7644769715	7.5461030763

TS 6^{Sc}-py^{Ph}-iqn to 7^{Sc}-py^{Ph}-iqn

Fe1	0.4783770102	1.1401544906	9.0264086155
Sc2	3.3388089407	2.1519470067	10.5400287123
Si3	3.2784216189	4.9515019036	8.4100659307
Si4	3.1196667573	-0.7643219070	12.5216367026
N5	2.5608811340	0.4132430805	11.3289366068
N6	2.7877714951	3.3418233287	8.9627682971
N7	5.6168799346	2.2750118442	10.6844913978
N8	3.6694544533	3.4918501527	12.1928711979
C9	6.0659089896	0.9092751288	8.6943801222
C10	7.9011588126	1.9527102954	9.9977817502
H11	8.6009372632	1.4903137559	9.3128323718
C12	1.0488275223	-0.7517864917	9.6365986715
H13	1.7929962935	-1.3551794978	9.1375257681
C14	2.9104805555	4.4620638607	12.6949828298
C15	4.4265062473	4.8028612526	14.5818690736
C16	6.5359783380	1.7470474276	9.8279979800
C17	1.3207724652	0.1725605568	10.7065302435
C18	6.0381672102	3.0447292223	11.7326631134
C19	3.3370538630	-2.4623382033	11.6948806660
H20	4.1014222379	-2.4227267928	10.9096270694
H21	2.4081322978	-2.8149802524	11.2359330920
H22	3.6555299849	-3.2215695849	12.4183072357
C23	8.3435246926	2.7266837226	11.0761115462
H24	9.4051924523	2.8972510466	11.2290592086
C25	4.4412855202	5.1016124551	15.9461517592
H26	3.8087171381	5.8910343480	16.3440642508
C27	1.9196272720	-0.9699808534	14.0291825904
C28	6.6348852234	1.0723296111	7.4196805779
H29	7.3716257595	1.8541067621	7.2611170671
C30	5.2868409962	4.3810512315	16.7919566660
H31	5.3170487134	4.6171320081	17.8521087007
C32	6.0719596044	3.0426440202	14.9238640622
H33	6.7014820840	2.2431257331	14.5421386323
C34	4.8176084497	-0.2058693150	13.1430558608
H35	5.5360196075	-0.0962992159	12.3237921238
H36	5.2262065230	-0.9554023516	13.8297378751
H37	4.7698640726	0.7462495417	13.6791917003
C38	5.0475956260	3.7026177960	12.5858840508

H39	4.7945387223	5.1436006682	12.5975211147
C40	3.4237599994	5.0658163858	6.4788019786
C41	1.4437074067	4.5502665548	12.3982026819
H42	1.1330673756	5.5976257389	12.3259093391
H43	0.8575185656	4.0956301836	13.2069440599
H44	1.1784595562	4.0477495132	11.4630269590
C45	5.2923493335	-0.7407408886	6.5489265205
H46	5.0010466045	-1.3846832182	5.7244126459
C47	0.0594068311	0.7973830862	11.0282824484
H48	-0.0759044402	1.5583728385	11.7839249088
C49	6.2502515860	0.2575342383	6.3575947024
H50	6.6979627906	0.4026549229	5.3787995691
C51	7.4162551328	3.2723939870	11.9396785700
H52	7.7173911470	3.8957305126	12.7722528411
C53	4.7180016419	-0.9071857093	7.8086603092
H54	3.9823914508	-1.6887598192	7.9734588514
C55	6.0929345653	3.3555230499	16.2853537722
H56	6.7427919610	2.7989693596	16.9547707379
C57	0.6609668987	-1.7751279501	13.6342629863
H58	-0.0203996314	-1.8566772166	14.4932355441
H59	0.9072372138	-2.7955661961	13.3214425514
H60	0.1040707130	-1.3007551751	12.8203835314
C61	3.6301445254	5.4240785046	13.4957654357
H62	3.1157599108	6.3579957724	13.7229189934
C63	5.2494316148	3.7795793120	14.0664960183
C64	4.1422420088	6.3839769791	6.1071411117
H65	4.1879197184	6.4927801634	5.0143237678
H66	5.1720995351	6.4129939878	6.4790392337
H67	3.6215689134	7.2665990934	6.4961492629
C68	5.0991372484	-0.0890730681	8.8746701487
H69	4.6692491481	-0.2662956003	9.8561984608
C70	0.2855795927	1.4645319524	7.0004317985
H71	-0.0462736482	0.7072807731	6.3030298229
C72	2.0335655113	5.0690856751	5.8035109011
H73	2.1444829368	5.1383254898	4.7117890333
H74	1.4265353465	5.9244131894	6.1201701696
H75	1.4662450273	4.1587019768	6.0155290503
C76	1.6319125703	1.7051965066	7.4001710747
H77	2.5102013705	1.1760382064	7.0562010437
C78	-0.3444583052	-0.7225525391	9.3425151574
H79	-0.8435496416	-1.2911617451	8.5693366713
C80	2.0412969056	6.2701856091	8.9885225437
H81	2.0601672993	6.3532005985	10.0803507159
H82	1.0156589938	6.0397331883	8.6847889011
H83	2.2894225492	7.2571128892	8.5810440080
C84	1.6463897241	2.7726755660	8.3669198334
C85	-0.9579178907	0.2390324828	10.2015339645
H86	-2.0020696839	0.5209586689	10.1968222157
C87	4.9530666096	5.3633073028	9.1842231777
H88	4.9227855586	5.2792726517	10.2745248439
H89	5.2247282637	6.3982388884	8.9486128848
H90	5.7552025537	4.7159732694	8.8149466785
C91	4.2442256046	3.8880879900	5.9166877582
H92	4.3937641131	4.0102809775	4.8340053172
H93	3.7408789480	2.9308404519	6.0714081562
H94	5.2378210502	3.8170943758	6.3745109636

C95	-0.5576343854	2.3607450674	7.7253796240
H96	-1.6375007470	2.3974745924	7.6743349918
C97	0.2687875830	3.1487784124	8.5762485739
H98	-0.0699540277	3.9036523380	9.2714060383
C99	2.6486811405	-1.7315645396	15.1602737401
H100	1.9589575869	-1.9172649036	15.9955760753
H101	3.4953096629	-1.1630009198	15.5592302628
H102	3.0241302489	-2.7077438351	14.8314265305
C103	1.4792516992	0.4050877069	14.5719795526
H104	0.8523897677	0.2788586285	15.4664697043
H105	0.8926689206	0.9635567930	13.8369176146
H106	2.3323995184	1.0301380485	14.8588821774
X107	0.2815208242	-0.1510431269	10.0667027123
X108	0.7179350676	2.2773451384	7.7716957752

I_N^{6-7}

Fe1	0.4549815428	1.2201227556	9.1319762595
Sc2	3.4095267185	2.1230781399	10.4180965272
Si3	3.3957163727	4.9021080056	8.2127774266
Si4	3.2088589183	-0.7150167091	12.5387942076
N5	2.6193500314	0.4789824596	11.3723741593
N6	2.8281815217	3.3704428180	8.8838433250
N7	5.5503143141	2.3217498110	10.7065135309
C8	6.0359266913	1.0636264220	8.6708484217
C9	7.8564293120	2.0061888806	10.0627946060
H10	8.5746228959	1.5709051929	9.3783221703
C11	1.0589366591	-0.6791863704	9.7187176554
H12	1.7925532279	-1.2763555999	9.1968694597
C13	2.5338587128	4.2355876125	12.8240143984
C14	3.9287479451	4.2901926277	14.8489818104
C15	6.5064123489	1.8416816603	9.8475181315
C16	1.3590403131	0.2397701222	10.7896594485
C17	5.9376462107	2.9871595039	11.8801254949
C18	3.2766368617	-2.4364068431	11.7274619842
H19	3.9871107826	-2.4501184093	10.8919980467
H20	2.3026369504	-2.7514216651	11.3395107539
H21	3.6070912621	-3.1969561644	12.4448230408
C22	8.2710331445	2.7298717416	11.2124508769
H23	9.3265417698	2.9323807382	11.3743797850
C24	3.9948941576	4.5463106630	16.2218094775
H25	3.1240123071	4.9782810454	16.7105945196
C26	2.1070282572	-0.8364066943	14.1293111872
C27	6.5969972524	1.2767590943	7.4007053394
H28	7.3335485388	2.0634078108	7.2717525410
C29	5.1351572090	4.2439857422	16.9620154880
H30	5.1774245427	4.4538273137	18.0264100596
C31	6.1537204829	3.3593324394	14.9438891423
H32	6.9793276496	2.8190782281	14.5015405165
C33	4.9716980032	-0.2468089083	13.0392456876
H34	5.6345837478	-0.1617421298	12.1720557994
H35	5.3866333251	-1.0247043243	13.6903103870
H36	5.0172834266	0.7017450281	13.5829506271
C37	4.9399472607	3.4896248570	12.7269969269
C38	3.4653448071	4.9350836734	6.2754544786
C39	1.2640069888	4.4683705687	12.0650286655

H40	0.4848717682	4.8356233711	12.7381977172
H41	0.8970234990	3.5550430059	11.5834351597
H42	1.3980049751	5.2091245642	11.2671754189
C43	5.2601893921	-0.5150457423	6.4707696773
H44	4.9677591407	-1.1284884304	5.6230249556
C45	0.1023269615	0.8507375556	11.1541085689
H46	-0.0215851495	1.5890142359	11.9329883559
C47	6.2153354916	0.4923910473	6.3142371063
H48	6.6600316191	0.6716160762	5.3392066194
C49	7.3449850230	3.1991062987	12.0979437806
H50	7.6550547042	3.8151067758	12.9309097086
C51	4.6921696226	-0.7344286436	7.7253165397
H52	3.9661717683	-1.5309069204	7.8646091498
C53	6.2022163684	3.6245934772	16.3089507925
H54	7.0831258265	3.3232656719	16.8705644357
C55	0.7620985799	-1.5370428075	13.8335989570
H56	0.1604689846	-1.6042133463	14.7520165971
H57	0.9054685752	-2.5600598284	13.4672155130
H58	0.1656886847	-0.9985034941	13.0912899438
C59	2.6914991217	4.5138619949	14.1240362076
H60	1.8352648637	4.8889374503	14.6779287613
C61	5.0412597842	3.7342225230	14.1486922210
C62	4.2183963491	6.2061574577	5.8170773136
H63	4.2183638436	6.2666172396	4.7192821855
H64	5.2647797988	6.2071206549	6.1410044399
H65	3.7517297097	7.1260515455	6.1883340345
C66	5.0787510009	0.0456876827	8.8180794324
H67	4.6812691119	-0.1933802785	9.8015381575
C68	0.1277253960	1.5588276908	7.1221121906
H69	-0.2779893973	0.8125527086	6.4520678299
C70	2.0452495293	4.9763329324	5.6681123032
H71	2.1051377718	5.0168342624	4.5706660403
H72	1.4863731120	5.8611994663	5.9931979517
H73	1.4568867672	4.0934662533	5.9310727372
C74	1.5056778987	1.7550263238	7.4242593632
H75	2.3377524055	1.1980934595	7.0171327845
C76	-0.3422248124	-0.6591345535	9.4693514260
H77	-0.8625402650	-1.2288314968	8.7108992460
C78	2.2787365712	6.3445539662	8.7613608587
H79	2.3969786230	6.5561743089	9.8305054754
H80	1.2193214361	6.1365058278	8.5786546988
H81	2.5283528900	7.2675921113	8.2253686141
C82	1.6263600558	2.8311836283	8.3800850804
C83	-0.9347287401	0.2896988141	10.3557730555
H84	-1.9821360356	0.5584903436	10.3907469827
C85	5.1326551792	5.2522312007	8.8909754562
H86	5.1715666830	5.3162675102	9.9846404515
H87	5.4839069873	6.2189124028	8.5128272998
H88	5.8591087162	4.4910854516	8.5909016328
C89	4.2140049477	3.7048180430	5.7254757913
H90	4.2775046388	3.7546285144	4.6284886613
H91	3.7119040377	2.7692836610	5.9845460545
H92	5.2386630062	3.6436626346	6.1085314054
C93	-0.6301284883	2.4842525191	7.9017931328
H94	-1.7091358509	2.5606865597	7.9241772864
C95	0.2789900514	3.2491941108	8.6856216724

H96	0.0133251785	4.0245618197	9.3892869076
C97	2.8532848269	-1.6677703326	15.1985662347
H98	2.2232367970	-1.7859623351	16.0918969284
H99	3.7842614188	-1.1884199988	15.5189389943
H100	3.0991158408	-2.6761980198	14.8441805752
C101	1.8309590228	0.5680939162	14.7043735852
H102	1.2327086273	0.4943042448	15.6243856472
H103	1.2764043435	1.1953325977	13.9996126463
H104	2.7544660201	1.1002492321	14.9591642184
N105	3.6423891436	3.7226521206	12.0341179088
H106	3.8214901258	4.4388894384	11.3169220455

TS 6^{Sc}-py^{Ph}-iqn to I_N^{6-7}

Fe1	0.5048601245	1.0982088702	8.9348102661
Sc2	3.3305538122	2.1365599354	10.4771052444
Si3	3.1205189946	5.0740659307	8.4997707983
Si4	3.0155781792	-0.6307434695	12.6298457396
N5	2.4994103476	0.4639440285	11.3476616546
N6	2.7189436960	3.4278983062	8.9887558694
N7	5.5573389990	2.1907030328	10.6491185993
N8	3.6798660044	3.4764717860	12.1401689103
C9	5.8908226970	0.8381908141	8.6236588879
C10	7.7916684437	1.9265386320	9.7679094565
H11	8.4439592327	1.4833615469	9.0256154874
C12	1.1646952433	-0.7734326645	9.5586291208
H13	1.9758628010	-1.3188333914	9.1003362357
C14	2.7501603368	4.1657036254	12.9592678339
C15	4.3770305454	4.4730914535	14.7870812164
C16	6.4311648663	1.7005990781	9.7082468136
C17	1.3130550137	0.1527372226	10.6544502255
C18	6.0619720074	2.9231891306	11.7126812430
C19	3.1233006540	-2.4102306011	11.9619393648
H20	3.9060284953	-2.4980092657	11.1987665571
H21	2.1813839042	-2.7355184783	11.5083578962
H22	3.3688040030	-3.1208288685	12.7600471224
C23	8.3106128212	2.7026827186	10.8285395462
H24	9.3737636867	2.9214470094	10.8765964400
C25	4.5941243351	4.8202589226	16.1226586263
H26	3.8167460606	5.3638821861	16.6545597196
C27	1.8401213163	-0.6382944343	14.1720550123
C28	6.3190971702	1.0202322701	7.2976159705
H29	6.9736991450	1.8533466201	7.0602614418
C30	5.7758591661	4.4655109625	16.7787187665
H31	5.9347645085	4.7568713756	17.8130715600
C32	6.5218412935	3.3526031878	14.7645226207
H33	7.2628679028	2.7354614106	14.2718124910
C34	4.7511428198	-0.1178216101	13.1842316392
H35	5.4425405401	-0.0520663398	12.3380222176
H36	5.1541940472	-0.8644652699	13.8777927995
H37	4.7649445838	0.8486242278	13.6980707762
C38	5.1501580620	3.5120538471	12.6342178481
H39	4.4985762381	4.3451724548	11.8779085143
C40	3.5981719560	5.2123356356	6.6247922286
C41	1.3604623854	4.2432416746	12.3970620404
H42	0.7182543363	4.8542526467	13.0360446437

H43	0.9156272997	3.2431341223	12.3285266258
H44	1.3593772289	4.6659581024	11.3872998182
C45	5.0517612764	-0.9134566857	6.5865945007
H46	4.7335156302	-1.5944656319	5.8021049128
C47	-0.0042792437	0.6861301648	10.9069477938
H48	-0.2400516710	1.4234721488	11.6606882262
C49	5.8999547503	0.1560666219	6.2888841669
H50	6.2346268186	0.3178276999	5.2678999117
C51	7.4632971314	3.1877317608	11.7876098652
H52	7.8326269421	3.8267551074	12.5786543173
C53	4.6222989275	-1.1056257155	7.8990512272
H54	3.9837917038	-1.9498060969	8.1435539778
C55	6.7281848676	3.7126300878	16.1011480947
H56	7.6365840480	3.3923440442	16.6041201414
C57	0.5273836505	-1.3968169677	13.8761906891
H58	-0.1236341957	-1.3897520394	14.7628803596
H59	0.7105493808	-2.4463381122	13.6191848733
H60	-0.0358905976	-0.9470396149	13.0527721032
C61	3.0891597239	4.7156329923	14.1453349301
H62	2.3302924434	5.2506919098	14.7084604149
C63	5.3824900418	3.7748054722	14.0663791038
C64	4.1677323311	6.6195325795	6.3322086806
H65	4.3941865513	6.7191829988	5.2607869542
H66	5.0976379937	6.8139656891	6.8776198196
H67	3.4586249963	7.4168114172	6.5846020535
C68	5.0323452513	-0.2349788092	8.9114420059
H69	4.7192960677	-0.4207400214	9.9341018437
C70	0.3460734045	1.4937223571	6.9131929371
H71	0.0633861938	0.7508021558	6.1792615215
C72	2.3647283301	5.0017147734	5.7175120368
H73	2.6539929255	5.0905230048	4.6599598763
H74	1.5881884170	5.7527113620	5.9024204948
H75	1.9129124635	4.0148838836	5.8512716996
C76	1.6716410681	1.7806580454	7.3502582963
H77	2.5799838269	1.3128754088	6.9962506994
C78	-0.2067024173	-0.8298792203	9.1815397736
H79	-0.6225897256	-1.4204279605	8.3760378429
C80	1.6753535670	6.2732835078	8.8097323376
H81	1.4356787361	6.3418565064	9.8769387227
H82	0.7645548483	5.9701941786	8.2840788353
H83	1.9284810404	7.2849989537	8.4710923415
C84	1.6180883004	2.8187429438	8.3517163417
C85	-0.9308923217	0.0735641160	10.0159910752
H86	-1.9899545600	0.2844575139	9.9558289848
C87	4.5753633709	5.6729836430	9.5587236506
H88	4.2462425411	5.8859617557	10.5827909846
H89	4.9803134750	6.6110626319	9.1648064048
H90	5.3977198101	4.9516481708	9.5999523752
C91	4.6703885455	4.1640894194	6.2663086613
H92	4.9594185342	4.2543538576	5.2086190919
H93	4.3117682274	3.1432660471	6.4261691334
H94	5.5811831769	4.2916123142	6.8647165650
C95	-0.5504661295	2.3256406965	7.6502747203
H96	-1.6292984819	2.3200654196	7.5730891020
C97	0.2201089472	3.1187190532	8.5473081028
H98	-0.1653145228	3.8319249944	9.2622969042

C99	2.5535080757	-1.3486631912	15.3455329650
H100	1.8826348966	-1.4114814864	16.2144893547
H101	3.4523815213	-0.8117263258	15.6667176375
H102	2.8482089853	-2.3745319253	15.0932237124
C103	1.5013852910	0.8023015326	14.6063597404
H104	0.8872311092	0.7943352032	15.5188796793
H105	0.9356563850	1.3333724273	13.8347272823
H106	2.3979565802	1.3944666419	14.8225334271

I_H^{6-7}

Sc1	4.8463071623	2.8490452165	4.1876351049
Fe2	3.3975544031	1.8885353184	7.0057029047
Si3	1.6327077843	4.1533006537	3.1969353990
Si4	7.1198143085	0.1030106141	4.5968921650
N5	6.0869988418	4.3207507180	2.5744875400
N6	4.7009673924	1.9795624849	1.9732672434
N7	2.8527682010	3.5051646149	4.2713616805
N8	5.7446142614	1.1213744034	4.9494729675
H9	5.8256941974	3.9648239741	5.2114766869
C10	6.3504824240	3.6211760015	1.4471768830
C11	7.5628559113	3.7235400665	0.7596240506
H12	7.7636105117	3.0838661250	-0.0906029907
C13	8.2001234975	5.4358552174	2.3021504321
C14	8.5120874190	4.6344214984	1.2154755469
H15	9.4695999224	4.7319043809	0.7117995373
H16	8.8819209773	6.2096909958	2.6347165514
C17	6.9746389116	5.2668980414	2.9714047694
C18	5.3114876822	2.6503489863	1.0004081227
C19	5.0065976057	2.4436869425	-0.3828666902
C20	4.1183906145	1.3662532134	-0.6932320299
C21	3.5704319668	0.6164228418	0.3712460675
H22	2.9095359674	-0.2172966069	0.1536354760
C23	3.8358693232	0.9532804180	1.6795528327
C24	2.4658692207	3.1864910485	5.5902658121
C25	1.5876462841	2.1251794976	6.0249114141
H26	1.1337103079	1.3885589942	5.3769706840
C27	1.4062878550	2.2229037431	7.4356908401
H28	0.8066381966	1.5624654883	8.0481052774
C29	2.2016526099	3.3120218311	7.9066581423
H30	2.3157282225	3.6137157512	8.9395512934
C31	2.8622340438	3.8925592716	6.7857288099
H32	3.5687425329	4.7109384487	6.8005781795
C33	5.1556463462	0.9802700306	6.2250950582
C34	4.1743193046	0.0002918537	6.6249493863
H35	3.7294838128	-0.7343340247	5.9683511797
C36	3.9026175188	0.1566174633	8.0151137178
H37	3.1993311363	-0.4254432410	8.5961120648
C38	4.6815284523	1.2535568440	8.4952446948
H39	4.6642958185	1.6507849171	9.5016961894
C40	5.4352469488	1.7698216721	7.4033630814
H41	6.0881426862	2.6302240064	7.4141067107
C42	0.4074131679	2.8105669257	2.6169937524
H43	0.9263725965	2.0339827577	2.0435178459
H44	-0.3736580358	3.2256154323	1.9688990178
H45	-0.0923634508	2.3217483562	3.4599927939

C46	2.4791764700	4.8119112150	1.6294727149
H47	2.9777148674	4.0072908964	1.0820777178
H48	3.2280386948	5.5815364683	1.8422453992
H49	1.7370258831	5.2478816777	0.9517645740
C50	0.5766441917	5.5940667272	3.9683556669
C51	-0.3449797459	5.0836897808	5.0982897445
H52	-0.9547657688	5.9112612129	5.4907031947
H53	0.2196763374	4.6666541617	5.9350725975
H54	-1.0385731360	4.3122154898	4.7444208375
C55	-0.3171730092	6.2259528526	2.8766466537
H56	-0.9383074602	7.0224770624	3.3120083540
H57	-1.0009491367	5.4967548035	2.4264702019
H58	0.2683582750	6.6785943624	2.0687618727
C59	1.4970399705	6.6916718493	4.5396808905
H60	0.9005041125	7.5079549299	4.9739315584
H61	2.1310902754	7.1341894540	3.7612720082
H62	2.1506480954	6.3024180026	5.3256800645
C63	6.6874636111	-1.7300612550	4.8746092012
H64	5.8971431133	-2.0508092318	4.1851465270
H65	6.3260322521	-1.9089689944	5.8924506169
H66	7.5515792953	-2.3844286559	4.7093018307
C67	7.5659432243	0.2977984706	2.7607502543
H68	6.7105313303	0.0546433483	2.1227645860
H69	8.3793420844	-0.3871747675	2.4967289177
H70	7.8975633150	1.3112026041	2.5103830894
C71	8.7058052413	0.5105673494	5.6429557267
C72	8.5411031374	0.0595604079	7.1116005022
H73	9.4511030966	0.2923423268	7.6848605139
H74	8.3787402825	-1.0217858330	7.1902941416
H75	7.7041460018	0.5571995611	7.6084678963
C76	9.9277610976	-0.2316475820	5.0560999885
H77	10.8209268707	-0.0358620885	5.6676753386
H78	10.1575829008	0.0908069044	4.0344787264
H79	9.7842040251	-1.3189685763	5.0387923910
C80	8.9851187219	2.0279347719	5.6080005501
H81	9.8726612670	2.2711409461	6.2119476524
H82	8.1421623343	2.6101973954	5.9917205622
H83	9.1828304027	2.3792445089	4.5868287104
C84	6.6330077785	6.2016554310	4.0674755973
C85	5.3361653399	6.7185582127	4.1882682452
C86	5.0456747795	7.6703620107	5.1616054448
C87	6.0408120032	8.1094691083	6.0365226820
C88	7.3333925910	7.5948906216	5.9291261906
C89	7.6306460701	6.6564530490	4.9441747147
H90	4.5580062281	6.3658098257	3.5212042182
H91	4.0379027967	8.0660305052	5.2404688569
H92	5.8094207635	8.8477706491	6.7995757903
H93	8.1103269043	7.9200456178	6.6157816973
H94	8.6319770230	6.2383937608	4.8890171607
C95	3.2273499217	0.2011097038	2.8273107431
H96	2.6051432131	0.8668594994	3.4338461057
H97	2.6094768567	-0.6240817061	2.4641203739
H98	4.0112061648	-0.1843234268	3.4856350798
C99	3.7930956838	1.0972433769	-2.0490795258
H100	3.1299602263	0.2657979839	-2.2716423293
C101	4.2911954324	1.8895684156	-3.0550366702

H102	4.0319547797	1.6828321518	-4.0894655689
C103	5.1201754932	2.9956055309	-2.7482207081
H104	5.4712400140	3.6411212228	-3.5477655052
C105	5.4706660693	3.2684018349	-1.4466970082
H106	6.0780763524	4.1378342103	-1.2278017336

2^{Sc}-imidazole

Sc1	-1.8596321151	6.3731094171	11.1690106965
Fe2	-1.9713365443	9.8568931605	11.4943371410
Si3	1.5897150666	6.8664214257	10.3667225986
N4	-1.1701894418	6.4073182209	13.4550703851
C5	0.0011431694	6.7084298259	13.9859550955
H6	0.8615310949	7.0522558038	13.4349160565
N7	-0.0025216091	6.5329014010	15.3335621311
C8	-1.2665865858	6.0851180889	15.6767515691
H9	-1.5376482478	5.8739483787	16.6999455644
C10	-1.9723742058	6.0124210627	14.5053826774
H11	-2.9969233556	5.7237235199	14.3409006833
C12	1.1137858242	6.7659084057	16.2357594405
H13	1.9639120947	7.1351121195	15.6599926980
H14	1.4057346055	5.8392519866	16.7389918962
H15	0.8494272929	7.5131918746	16.9899159900
N16	-0.0403477125	7.3740832033	10.7481433832
C17	-0.2597019171	8.7624455780	10.8193547264
C18	-0.7929373565	9.6165305431	9.7851884613
H19	-1.1156788958	9.2694806451	8.8146826045
C20	-3.9995462707	9.6104714196	11.1051932281
H21	-4.4670893297	9.4602202576	10.1439352690
C22	-3.7566158607	10.8731021467	11.7210924156
H23	-3.9561674754	11.8447856529	11.2885125862
C24	-3.1579725477	10.6278425183	12.9928115547
H25	-2.8158082969	11.3819760597	13.6890633842
C26	1.9513404597	5.1341217737	11.0572245041
H27	1.6459981203	5.0593745550	12.1069127375
H28	3.0284935807	4.9347915886	11.0112337780
H29	1.4330879602	4.3376889541	10.5198618822
C30	2.8684308911	8.0187177725	11.1975524731
H31	2.7166663061	9.0712412983	10.9415340904
H32	3.8859468671	7.7433838736	10.8953266703
H33	2.8317087738	7.9455489486	12.2918267131
C34	1.9900374006	6.8748260039	8.4645984040
C35	2.1209548215	8.3212034440	7.9388096265
H36	2.3208202668	8.3182292471	6.8569214274
H37	2.9461475041	8.8600198124	8.4181661514
H38	1.2090363738	8.9039983130	8.1028804256
C39	3.3229771962	6.1413793559	8.1986024501
H40	3.2770352676	5.0862938477	8.4890738454
H41	4.1623462255	6.5980400216	8.7367759014
H42	3.5713185274	6.1755412408	7.1275627047
C43	0.8674649166	6.1658387232	7.6808243410
H44	-0.0992602113	6.6551726250	7.8298138624
H45	0.7520399569	5.1212884776	7.9910643880
H46	1.0892816285	6.1663594892	6.6025821084
Si47	-5.3663367229	6.5457325277	11.7836230784
N48	-2.8094581116	6.4781726956	8.9238665849

C49	-3.2783935105	7.5381531466	8.2841689478
H50	-3.1994873903	8.5578832033	8.6274289741
N51	-3.9007789901	7.1902827434	7.1286607429
C52	-3.8276803009	5.8134162198	7.0315282859
H53	-4.2528110210	5.2780227829	6.1969806474
C54	-3.1468850698	5.3905277389	8.1416024865
H55	-2.8709132499	4.3900218600	8.4319487113
C56	-4.5827744533	8.0890370990	6.2112108964
H57	-4.3568228625	9.1201833878	6.4887479327
H58	-5.6658787578	7.9410588786	6.2583635985
H59	-4.2408596095	7.9190459974	5.1867934830
N60	-1.2701316882	4.3645501158	10.3847506807
C61	-1.9439734274	4.1645029887	11.5301329156
N62	-1.9433417444	2.8178813900	11.7728853358
C63	-1.2663132061	2.1676650057	10.7508522136
H64	-1.1393905746	1.0947384413	10.7351700489
C65	-0.8525974586	3.1440505494	9.8862727550
H66	-0.2857460203	3.0442132594	8.9702297743
C67	-2.5627881232	2.1646077758	12.9112614671
H68	-3.4375050950	1.5777874798	12.6093254819
H69	-2.8795036536	2.9355416832	13.6135572604
H70	-1.8492612514	1.5018956764	13.4121095539
N71	-3.7338835526	7.1640393623	11.8200490532
C72	-3.5941409607	8.5503759728	12.0046078391
C73	-3.0400541563	9.2166665907	13.1584970150
H74	-2.6022296051	8.7090486339	14.0044699662
C75	0.0392413267	9.6386245932	11.9274428611
H76	0.4175506667	9.3147879032	12.8856119248
C77	-0.2462089073	10.9848717363	11.5575194859
H78	-0.1336403549	11.8579231093	12.1869068530
C79	-0.7703497729	10.9712405615	10.2303841756
H80	-1.1126195698	11.8334075267	9.6737071056
C81	-5.3320675423	4.6502206929	11.7150029012
H82	-4.7060638235	4.3004463388	10.8888285197
H83	-6.3451737507	4.2615612001	11.5591859423
H84	-4.9362561811	4.2042003820	12.6327421024
C85	-6.3420556832	7.0929057894	10.2338707140
H86	-6.4336799118	8.1807272629	10.1533229650
H87	-7.3573938645	6.6778905996	10.2387446376
H88	-5.8434385190	6.7275295886	9.3291115879
C89	-6.4338387131	7.0731493712	13.3295895013
C90	-6.8044579635	8.5724784919	13.2883494399
H91	-7.4310673399	8.8319135749	14.1552716368
H92	-7.3775975921	8.8278985730	12.3899696680
H93	-5.9230137505	9.2179562497	13.3161579848
C94	-7.7479496980	6.2588417668	13.3502878311
H95	-7.5670154079	5.1835367901	13.4561620122
H96	-8.3434292798	6.4082972960	12.4421813095
H97	-8.3739199946	6.5690832478	14.2000417369
C98	-5.6750819793	6.7961981058	14.6432140185
H99	-4.7565622696	7.3860850598	14.7110644839
H100	-5.4080740007	5.7363499937	14.7445564028
H101	-6.2995827598	7.0539985816	15.5117372547
X102	-1.7335000000	4.0700000000	11.0735000000
X103	-0.5142000000	9.9066000000	10.4260000000
X104	-3.4208000000	9.9066000000	12.0290000000

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Sc1	-1.8596321151	6.3731094171	11.1690106965
Fe2	-1.9713365443	9.8568931605	11.4943371410
Si3	1.5897150666	6.8664214257	10.3667225986
N4	-1.1701894418	6.4073182209	13.4550703851
C5	0.0011431694	6.7084298259	13.9859550955
H6	0.8615310949	7.0522558038	13.4349160565
N7	-0.0025216091	6.5329014010	15.3335621311
C8	-1.2665865858	6.0851180889	15.6767515691
H9	-1.5376482478	5.8739483787	16.6999455644
C10	-1.9723742058	6.0124210627	14.5053826774
H11	-2.9969233556	5.7237235199	14.3409006833
C12	1.1137858242	6.7659084057	16.2357594405
H13	1.9639120947	7.1351121195	15.6599926980
H14	1.4057346055	5.8392519866	16.7389918962
H15	0.8494272929	7.5131918746	16.9899159900
N16	-0.0403477125	7.3740832033	10.7481433832
C17	-0.2597019171	8.7624455780	10.8193547264
C18	-0.7929373565	9.6165305431	9.7851884613
H19	-1.1156788958	9.2694806451	8.8146826045
C20	-3.9995462707	9.6104714196	11.1051932281
H21	-4.4670893297	9.4602202576	10.1439352690
C22	-3.7566158607	10.8731021467	11.7210924156
H23	-3.9561674754	11.8447856529	11.2885125862
C24	-3.1579725477	10.6278425183	12.9928115547
H25	-2.8158082969	11.3819760597	13.6890633842
C26	1.9513404597	5.1341217737	11.0572245041
H27	1.6459981203	5.0593745550	12.1069127375
H28	3.0284935807	4.9347915886	11.0112337780
H29	1.4330879602	4.3376889541	10.5198618822
C30	2.8684308911	8.0187177725	11.1975524731
H31	2.7166663061	9.0712412983	10.9415340904
H32	3.8859468671	7.7433838736	10.8953266703
H33	2.8317087738	7.9455489486	12.2918267131
C34	1.9900374006	6.8748260039	8.4645984040
C35	2.1209548215	8.3212034440	7.9388096265
H36	2.3208202668	8.3182292471	6.8569214274
H37	2.9461475041	8.8600198124	8.4181661514
H38	1.2090363738	8.9039983130	8.1028804256
C39	3.3229771962	6.1413793559	8.1986024501
H40	3.2770352676	5.0862938477	8.4890738454
H41	4.1623462255	6.5980400216	8.7367759014
H42	3.5713185274	6.1755412408	7.1275627047
C43	0.8674649166	6.1658387232	7.6808243410
H44	-0.0992602113	6.6551726250	7.8298138624
H45	0.7520399569	5.1212884776	7.9910643880
H46	1.0892816285	6.1663594892	6.6025821084
Si47	-5.3663367229	6.5457325277	11.7836230784
N60	-1.2701316882	4.3645501158	10.3847506807
C61	-1.9439734274	4.1645029887	11.5301329156
N62	-1.9433417444	2.8178813900	11.7728853358
C63	-1.2663132061	2.1676650057	10.7508522136
H64	-1.1393905746	1.0947384413	10.7351700489
C65	-0.8525974586	3.1440505494	9.8862727550

H66	-0.2857460203	3.0442132594	8.9702297743
C67	-2.5627881232	2.1646077758	12.9112614671
H68	-3.4375050950	1.5777874798	12.6093254819
H69	-2.8795036536	2.9355416832	13.6135572604
H70	-1.8492612514	1.5018956764	13.4121095539
N71	-3.7338835526	7.1640393623	11.8200490532
C72	-3.5941409607	8.5503759728	12.0046078391
C73	-3.0400541563	9.2166665907	13.1584970150
H74	-2.6022296051	8.7090486339	14.0044699662
C75	0.0392413267	9.6386245932	11.9274428611
H76	0.4175506667	9.3147879032	12.8856119248
C77	-0.2462089073	10.9848717363	11.5575194859
H78	-0.1336403549	11.8579231093	12.1869068530
C79	-0.7703497729	10.9712405615	10.2303841756
H80	-1.1126195698	11.8334075267	9.6737071056
C81	-5.3320675423	4.6502206929	11.7150029012
H82	-4.7060638235	4.3004463388	10.8888285197
H83	-6.3451737507	4.2615612001	11.5591859423
H84	-4.9362561811	4.2042003820	12.6327421024
C85	-6.3420556832	7.0929057894	10.2338707140
H86	-6.4336799118	8.1807272629	10.1533229650
H87	-7.3573938645	6.6778905996	10.2387446376
H88	-5.8434385190	6.7275295886	9.3291115879
C89	-6.4338387131	7.0731493712	13.3295895013
C90	-6.8044579635	8.5724784919	13.2883494399
H91	-7.4310673399	8.8319135749	14.1552716368
H92	-7.3775975921	8.8278985730	12.3899696680
H93	-5.9230137505	9.2179562497	13.3161579848
C94	-7.7479496980	6.2588417668	13.3502878311
H95	-7.5670154079	5.1835367901	13.4561620122
H96	-8.3434292798	6.4082972960	12.4421813095
H97	-8.3739199946	6.5690832478	14.2000417369
C98	-5.6750819793	6.7961981058	14.6432140185
H99	-4.7565622696	7.3860850598	14.7110644839
H100	-5.4080740007	5.7363499937	14.7445564028
H101	-6.2995827598	7.0539985816	15.5117372547
X102	-1.6070525578	4.2645265523	10.9574417982
X103	-0.4059913254	9.9947426024	10.8639779421
X104	-3.5096659592	9.7756917296	12.1964404105

TS 2^{Sc}-imidazole to 3^{Sc}-imidazole

Sc	-1.7476978510	6.6696973356	11.3993418058
Si	1.5704129271	7.1828104946	10.3421888626
N	-0.8553656786	6.6059836743	13.5173068963
C	-0.6779349483	5.2810377365	13.8182065753
H	0.1362212650	4.7182543851	13.3766864606
N	-0.8968137859	5.0847828153	15.1657169311
C	-1.3944651461	6.2826018744	15.6911365049
H	-1.7245083246	6.3665675073	16.7148310785
C	-1.3533869737	7.1821729366	14.6684254331
H	-1.6357373143	8.2225924533	14.6881215262
C	-0.4750622150	3.9375317971	15.9411673607
H	-0.0027472851	3.2092561356	15.2774294682
H	-1.3214439468	3.4469605988	16.4395850642
H	0.2535701186	4.2292316492	16.7085200112

N	-0.0847523548	7.6835006463	10.6554436827
C	-0.2719832944	9.0692179394	10.8263463687
C	-0.6446833304	10.0291360715	9.8159058212
H	-0.8739000434	9.7833610157	8.7882968718
C	-3.9128297859	9.7306783034	10.6827636539
H	-4.1698956613	9.3966644398	9.6880542080
C	-3.8380001012	11.0857488846	11.1180263974
H	-3.9841723104	11.9635234216	10.5030545073
C	-3.4804665314	11.0831754026	12.4983253297
H	-3.3112198059	11.9580681238	13.1117893872
C	2.0799681430	5.7480563154	11.4735853658
H	2.0089640867	6.0739617002	12.5166625822
H	3.1142387663	5.4383874772	11.2874150825
H	1.4356374183	4.8734477001	11.3483033589
C	2.7702217047	8.6127084357	10.6977142904
H	2.5899433194	9.4817991333	10.0579311975
H	3.8072548183	8.2940487290	10.5467623174
H	2.6766993341	8.9503075286	11.7339741867
C	1.8443193918	6.6318082901	8.4983978541
C	1.3019229037	7.7048596694	7.5338281420
H	1.4854959000	7.4160361898	6.4899358139
H	1.7806618272	8.6754386336	7.6870220292
H	0.2244612881	7.8417887586	7.6566851500
C	3.3516873409	6.4346595107	8.2163003676
H	3.8096951109	5.7008669824	8.8913477759
H	3.9160020420	7.3689106467	8.3106115867
H	3.5044060000	6.0689605799	7.1923355504
C	1.1165169913	5.3034339660	8.2159123784
H	0.0408721808	5.3838606124	8.4031237788
H	1.5103949601	4.4879120299	8.8318002547
H	1.2497231009	5.0085623289	7.1652886466
Si	-5.2546574468	6.7157631502	11.8772497281
N	-2.5270020831	6.2571004807	9.1369888729
C	-2.7616970280	7.2383044841	8.2776866590
H	-2.5605176895	8.2852819044	8.4583560830
N	-3.2957499313	6.7715016431	7.1186005976
C	-3.4067618196	5.3990536156	7.2513407505
H	-3.8095765437	4.7808847106	6.4631739099
C	-2.9242846502	5.0968272319	8.4993997904
H	-2.8401056375	4.1333777219	8.9802638311
C	-3.7052109628	7.5690707234	5.9696790379
H	-3.5007307286	8.6217417381	6.1761993271
H	-4.7778980400	7.4500340804	5.7813777182
H	-3.1472114893	7.2727249732	5.0757555603
N	-1.2496643339	4.5292167471	11.2888539232
C	-1.8168601349	4.2941498008	12.5032390672
N	-1.9219184953	2.9285715407	12.6202745506
C	-1.4014957289	2.3132969324	11.4891096069
H	-1.3798863481	1.2404543697	11.3711151015
C	-0.9887847375	3.3225719290	10.6658106757
H	-0.5289575331	3.2602667000	9.6896791047
C	-2.5905064810	2.2365000883	13.7067660653
H	-3.5189359553	1.7731268907	13.3616362941
H	-2.8355493151	2.9678986529	14.4738899339
H	-1.9509077402	1.4588291091	14.1338470814
N	-3.6570157223	7.4463665617	11.8045400164

C	-3.6266295573	8.8567671220	11.7968234757
C	-3.3419864239	9.7275328558	12.9113062949
H	-3.0840555410	9.3899077353	13.9023178382
C	-0.0610766304	9.8286560450	12.0355496782
H	0.2113909130	9.3925472692	12.9860464509
C	-0.2641908772	11.2105011494	11.7586276812
H	-0.2031671939	12.0213595883	12.4722867635
C	-0.6254153467	11.3361829244	10.3837723704
H	-0.8786870306	12.2578478465	9.8768148539
C	-5.1176709015	4.8447736953	11.5975200929
H	-4.6165927747	4.6247350902	10.6496197783
H	-6.1185023316	4.3994574786	11.5482649721
H	-4.5578729934	4.3489820845	12.3963038480
C	-6.3836200916	7.3895185559	10.4961818369
H	-6.5273804075	8.4728065617	10.5672370157
H	-7.3743346776	6.9189529392	10.5289390014
H	-5.9512402771	7.1763451701	9.5104812205
C	-6.1818534274	6.9958582810	13.5673570152
C	-6.7247548017	8.4483346066	13.6867554875
H	-7.2499036512	8.5733512977	14.6449688214
H	-7.4453924702	8.6853279625	12.8840274893
H	-5.9276040325	9.2057015063	13.6568308582
C	-7.3888835215	6.0223889276	13.6587146663
H	-7.0813998036	4.9645114622	13.6624304398
H	-8.1052932227	6.1576389851	12.8298122679
H	-7.9380881267	6.2001610849	14.5941013328
C	-5.2246060434	6.7241900547	14.7620256432
H	-4.3593240475	7.3992298452	14.7684004736
H	-4.8330775436	5.6933251409	14.7442993195
H	-5.7505394356	6.8565690379	15.7185745757
Fe	-2.0029327829	10.1619881586	11.3771077345

TS 2^{Sc} to 3^{Sc}

Sc	-1.5964706673	6.8281665772	11.8790461658
Si	1.4572213641	7.1229451119	10.1084317337
N	-0.7844814366	6.8414843958	13.9300101442
C	-0.5397517707	5.4942542401	14.0746220116
H	0.2981318842	5.0303701294	13.5622543404
N	-0.7412629125	5.1440136620	15.3918384151
C	-1.3529575041	6.2332502994	16.0297040438
H	-1.6789073295	6.1814385266	17.0568801001
C	-1.3721268203	7.2428747068	15.1196256012
H	-1.7386125566	8.2504932305	15.2459607436
C	-0.1783970553	3.9905298548	16.0636701699
H	0.2239804028	3.2999469169	15.3192510738
H	-0.9387294267	3.4605469956	16.6483606558
H	0.6345461006	4.2859310006	16.7392021561
N	-0.0479770191	7.6793999218	10.8164377178
C	-0.1896641895	9.0719966104	11.0026463478
C	-0.5399700164	10.0613564735	10.0156413179
H	-0.7917832254	9.8468307880	8.9871865211
C	-3.7608809180	9.7640946695	10.6960753564
H	-3.8953120189	9.4767779724	9.6629440806
C	-3.7265447278	11.0961618349	11.2038568202
H	-3.8260652665	12.0010568927	10.6199140264

C	-3.4755392210	11.0300133253	12.6073949665
H	-3.3551837392	11.8751439652	13.2719943763
C	2.0994657813	5.6277219329	11.0900382160
H	2.3042257557	5.9358379870	12.1225485994
H	3.0330995127	5.2340388953	10.6719674569
H	1.3707459216	4.8118616064	11.1173124389
C	2.7634040951	8.4956307238	10.2369822575
H	2.5060713778	9.3731030544	9.6348974249
H	3.7473883525	8.1408629779	9.9110395791
H	2.8575978710	8.8332795957	11.2748044437
C	1.2815555335	6.6158898640	8.2442974950
C	0.6781618297	7.7709280709	7.4187961722
H	0.6284031390	7.4990251550	6.3539362176
H	1.2730813006	8.6888286524	7.4912109136
H	-0.3405245360	8.0035722807	7.7456738925
C	2.6715986582	6.2693757130	7.6664653410
H	3.1565288367	5.4528901025	8.2141336144
H	3.3485767935	7.1304042911	7.6848401520
H	2.5828040845	5.9486378747	6.6181282782
C	0.3633038360	5.3856510470	8.0983941754
H	-0.6365772217	5.5801876517	8.5035656846
H	0.7734943668	4.5085569758	8.6123087897
H	0.2425262740	5.1161951518	7.0385582892
Si	-5.1130688541	6.6398772622	11.4812533444
N	-1.3196342673	4.7148043783	11.4685448671
C	-1.7172984982	4.5573691667	12.7571877921
N	-1.9961980458	3.2284695176	12.9246260373
C	-1.7723693411	2.5537773007	11.7299789276
H	-1.9453317109	1.4927795788	11.6287578799
C	-1.3549816583	3.4920471894	10.8310363904
H	-1.0926688733	3.3730285197	9.7899852307
C	-2.6194053589	2.6362929693	14.0994713859
H	-3.6140688855	2.2537250291	13.8495237532
H	-2.7280707050	3.4093949322	14.8596744142
H	-2.0146072450	1.8131323798	14.4939085251
N	-3.5648534862	7.4331439304	11.7356597165
C	-3.5646266573	8.8443275073	11.7875793415
C	-3.3721537935	9.6557006576	12.9662608320
H	-3.1982390239	9.2640357768	13.9575473777
C	0.0219194214	9.7916741855	12.2374690073
H	0.2807151672	9.3231374189	13.1768697089
C	-0.1760043290	11.1817813566	12.0021519275
H	-0.1120794428	11.9701666551	12.7405791777
C	-0.5118009456	11.3500687788	10.6243382456
H	-0.7485349284	12.2878658311	10.1390877000
C	-4.8176089639	4.8224198859	11.0410927129
H	-4.1214286385	4.7293833565	10.2013782940
H	-5.7606297374	4.3518984565	10.7409215294
H	-4.4068975143	4.2469174405	11.8751303965
C	-6.0567721488	7.4098217590	10.0213968966
H	-6.2696691749	8.4722051507	10.1716828187
H	-7.0133651340	6.8991406453	9.8584693185
H	-5.4747405761	7.3169820545	9.0971439676
C	-6.2506958446	6.7271986579	13.0511857070
C	-6.7776659132	8.1613917764	13.2760321586
H	-7.4091395654	8.1977744046	14.1750329629

H	-7.3903275444	8.5095448476	12.4379449645
H	-5.9673538551	8.8831105685	13.4159910970
C	-7.4637668041	5.7889267373	12.8710081794
H	-7.1624163632	4.7392569935	12.7765614768
H	-8.0589171595	6.0452167669	11.9861305966
H	-8.1338296377	5.8599050771	13.7409801945
C	-5.4669330397	6.2889437402	14.3048034779
H	-4.6022024231	6.9320914129	14.4917950127
H	-5.0936500308	5.2617805364	14.2143435494
H	-6.1117072601	6.3252044109	15.1956202163
Fe	-1.9211448246	10.1552027899	11.5467295072

3^{Sc}-imidazole

Sc	11.0970746921	11.1889337823	12.8349722138
N	12.4063739078	12.6276603869	13.6727014231
N	9.3287489662	11.2880746631	11.7297144826
Fe	10.1062836959	14.3733752712	12.2230957822
Si	8.0348885635	10.1460905873	11.4033916001
Si	13.4213341820	12.4906002431	15.0883159967
N	11.9112871802	9.0318867398	12.8745908304
N	10.4152904829	10.2938492823	14.6426803672
N	9.5202418246	8.2544756147	15.3848918506
N	12.4422436982	7.2427685598	14.0513669554
C	12.2068581982	10.7262060443	9.6338087474
C	9.0653337590	12.6493794898	11.5087915384
C	10.6373076078	15.8750294873	13.5356700274
H	9.9492650142	16.6356020327	13.8805619236
C	12.1552880032	14.7170856737	12.2389992740
H	12.8282516476	14.4486243824	11.4367566932
C	8.9952387843	14.7689227175	10.5288636031
H	9.1929776490	15.6044344151	9.8701535814
C	8.1580465077	14.7952204909	11.6858490137
H	7.6112662620	15.6536663568	12.0531785408
C	10.8629333700	14.6064060107	14.1446567847
H	10.3954146021	14.2372936656	15.0472420202
C	9.5677580452	13.4674650316	10.4304567680
H	10.2667467876	13.1302148768	9.6778451166
C	11.8460366185	13.8786471332	13.3729730657
C	8.2178509026	13.5113132774	12.3000675990
H	7.7103357694	13.2110780447	13.2060575737
C	11.4363033528	15.9426931458	12.3538158493
H	11.4559133096	16.7624819409	11.6476555200
C	8.6767134938	8.3970801062	11.7373017649
H	8.9412112843	8.2781724874	12.7926358539
H	9.5589824510	8.1498537648	11.1365322840
H	7.8993551553	7.6587731041	11.5092945410
C	6.5837120742	11.5210354654	9.3085902810
H	6.2224055789	11.5466021202	8.2691860452
H	7.1787583131	12.4243409801	9.4712956152
H	5.7028069494	11.5806070951	9.9573575026
C	8.5692779475	10.1846610824	8.5637517365
H	8.1996734543	10.1745908332	7.5271844664
H	9.1805154481	9.2818994399	8.6953594560
H	9.2206870702	11.0574623578	8.6708452311
C	14.2914259267	10.8010531380	15.0153453464

H	13.5633983783	9.9853664750	14.9961893235
H	14.9243926862	10.6526673275	15.8973015127
H	14.9262156060	10.6957785077	14.1279816313
C	6.5222035353	10.4332911224	12.5204388629
H	6.8042238972	10.2729219717	13.5659713629
H	5.7081909418	9.7376919730	12.2827730693
H	6.1243798923	11.4490240053	12.4263293312
C	6.4744768549	9.0227776762	9.2827306074
H	6.0589059517	9.0872230965	8.2660484772
H	5.6250942481	8.9806211710	9.9744689990
H	7.0099913357	8.0697648593	9.3547361186
C	12.4472251841	12.5529767915	16.7185911534
H	11.6512731041	11.8015214987	16.6805622311
H	11.9764290431	13.5283460221	16.8828926464
H	13.0795831595	12.3416387205	17.5894216755
N	12.4589304731	11.2023877661	10.9049743146
N	14.2389994853	11.5697645400	9.6438563586
H	11.2588144109	10.2784409000	9.3815567836
C	13.3010683129	10.9461826528	8.8397052717
H	13.4928426629	10.7350992339	7.7986927467
C	12.8151313313	8.2869494392	12.1492925423
C	13.1497100156	7.1722371451	12.8622804585
H	13.1582144541	8.6032967050	11.1770381161
C	9.1504955867	10.4869144602	15.2011439332
C	10.7964403963	8.9645123361	15.0854867549
H	11.3935198826	8.9987638836	16.0413343138
C	7.3961567347	10.2316581556	9.5621220413
C	14.8097736138	13.8555232107	15.1501993436
C	15.5796352407	13.9040096328	13.8138141453
H	16.3995573123	14.6363838495	13.8623399795
H	14.9249072041	14.2009637948	12.9875190718
H	16.0299075683	12.9337473617	13.5652063685
C	15.8094563006	13.5207615651	16.2806158982
H	16.5799438946	14.3027417845	16.3525520140
H	16.3273806953	12.5702012418	16.1105765260
H	15.3185578716	13.4625797214	17.2590813310
C	14.2259084102	15.2576912134	15.4328201704
H	15.0346120954	16.0020427668	15.4890269311
H	13.6915406679	15.2907170816	16.3890073763
H	13.5325378832	15.5839600587	14.6533050522
C	11.6847853396	8.3744137720	14.0124403448
C	9.5832518590	7.2214703439	16.4027498889
H	8.5703193803	6.9874366914	16.7413623979
H	10.1732470713	7.5322485391	17.2887038777
H	10.0086602533	6.2955642138	16.0057710383
C	12.5674373294	6.2730967919	15.1314795285
H	12.3360431507	6.7506651504	16.0834852473
H	13.5983945477	5.9129730261	15.1635834016
H	11.8967083194	5.4222475765	14.9811032431
C	8.6239835783	9.3421210210	15.6721732471
H	8.6709410579	11.4567846549	15.1568706555
H	7.6406280740	9.1396326849	16.0717993111
H	13.8120896644	6.3472449248	12.6488422022
C	15.5610208569	12.0243343859	9.2390157167
H	16.0553429514	12.4831919779	10.0967321949
H	15.4824217792	12.7658060506	8.4387511579

H	16.1664006324	11.1829934593	8.8896852943
C	13.6854744901	11.7014057352	10.8759427517
H	14.1748563746	12.1680685601	11.7185372762

3^{Sc}

Sc	10.6605141083	11.3667510703	13.4004798370
N	11.9815312589	12.7807204711	14.1346588049
N	9.2120502694	11.3483199205	11.9341142002
Fe	9.9273837933	14.4509752851	12.3330585409
Si	8.1222250397	10.0992005332	11.3343784546
Si	13.2466247952	12.7655332779	15.3499340538
N	11.9177858041	9.5621791210	12.9908230429
N	10.1245091288	10.0477003361	14.9222934795
N	9.7327426420	7.7405813616	15.1397803926
N	12.8093095082	7.7141737212	13.7904405913
C	8.9540552486	12.6921425378	11.6162111170
C	10.4221950723	16.0720914014	13.5214475817
H	9.7478750540	16.8923296889	13.7285917324
C	11.9781420605	14.7229634835	12.4774368390
H	12.6977809801	14.3382690738	11.7675570789
C	8.9636970414	14.7617847043	10.5390246069
H	9.2165760358	15.5671442239	9.8627725226
C	8.0247007875	14.8335971315	11.6129093814
H	7.4423616991	15.7025543766	11.8888013099
C	10.5452482179	14.8736723959	14.2802810613
H	10.0059597606	14.6254866267	15.1845549948
C	9.5528775889	13.4642878050	10.5548600074
H	10.3196944618	13.1009357776	9.8847719830
C	11.5371112648	14.0266979456	13.6605491708
C	8.0280500717	13.5772776286	12.2831849540
H	7.4323784308	13.3073945707	13.1449999586
C	11.3108216825	15.9800864608	12.4068915268
H	11.4235603742	16.7177331720	11.6233953117
C	8.8755345770	8.4041565257	11.7028683607
H	9.0604373698	8.2573629976	12.7701634359
H	9.8217766526	8.2539932766	11.1710431700
H	8.1859711931	7.6141761735	11.3830014858
C	6.9740075005	11.4356912088	9.0294622216
H	6.7831646649	11.4408686987	7.9458033051
H	7.4778545567	12.3737624479	9.2771072662
H	5.9979980832	11.4386016814	9.5282139116
C	9.1490887583	10.2263496704	8.6493419276
H	8.9705700263	10.2373102495	7.5640428348
H	9.7645478576	9.3451700371	8.8675871940
H	9.7417683514	11.1124846592	8.8942647076
C	13.2761267569	11.0582137118	16.1710420771
H	12.2682382834	10.7965272926	16.5081618227
H	13.9372627530	11.0678863505	17.0446062409
H	13.6296684155	10.2689583500	15.4984229327
C	6.4460753671	10.2187696301	12.2240294965
H	6.5834092065	9.9934059821	13.2877298527
H	5.7121115422	9.5076816452	11.8268503115
H	6.0130525336	11.2219287875	12.1443626065
C	7.0280372330	8.9394370122	8.9728919866
H	6.8043143978	8.9946156749	7.8974699244

H	6.0692640418	8.8406395901	9.4954115316
H	7.5954220428	8.0175009217	9.1388790409
C	12.8956508168	14.0422562634	16.7125351536
H	11.9805123851	13.7768318842	17.2546211822
H	12.7591055695	15.0506830802	16.3093471093
H	13.7113763474	14.0836171267	17.4441792369
C	12.9674228343	9.2033849925	12.1743051359
C	13.5273912045	8.0555585738	12.6550776923
H	13.2508923496	9.7937691379	11.3161740944
C	8.8223405728	9.8071802137	15.3817845881
C	10.8117764026	8.7684590069	15.0806509772
H	11.3822005380	8.7210390405	16.0453465737
C	7.8110470903	10.1972407887	9.4178010973
C	15.0073153884	13.1214763838	14.6104054424
C	15.2221596643	12.3059201743	13.3186773818
H	16.2309935885	12.4783972287	12.9147477621
H	14.5011030409	12.5841675840	12.5427489582
H	15.1192749716	11.2270727746	13.4900720475
C	16.0898623057	12.7164422857	15.6359844757
H	17.0913538164	12.9584244162	15.2512546622
H	16.0740239814	11.6420436160	15.8499474661
H	15.9756727184	13.2469053509	16.5890745122
C	15.1847129816	14.6217407925	14.2903537863
H	16.1808075018	14.8069291281	13.8614890413
H	15.0997288520	15.2422322541	15.1895462727
H	14.4445745689	14.9825365310	13.5695098668
C	11.8244256407	8.6402047231	13.9533186497
C	10.0086567314	6.5610509278	15.9430286440
H	9.0689220900	6.0438819695	16.1536461056
H	10.4847811032	6.8081688140	16.9122069383
H	10.6486040623	5.8539425644	15.4088302761
C	13.1299957997	6.5728483402	14.6390416974
H	12.8180312838	6.7754362754	15.6635124948
H	14.2114897863	6.4211055196	14.6280004041
H	12.6382102018	5.6637198965	14.2820455397
C	8.5812551861	8.4960813752	15.5401378793
H	8.1211314516	10.6230808279	15.5044291066
H	7.6661565241	7.9841721810	15.8008990574
H	14.3559523148	7.4562010797	12.3104593328

TS 3^{Sc}-imidazole to I$_{Sc}$$^{3-4}$-imidazole

Sc1	10.9688662448	11.0189875697	13.0592705787
N2	12.2996174780	12.5644621430	13.6799356418
N3	9.2801224753	11.1123542960	11.7623124247
Fe4	9.8941562138	14.2397007438	12.3433452833
Si5	8.0870249862	10.0131215838	11.1147988269
Si6	13.6781820251	12.6280045348	14.7778396859
N7	12.0933149621	8.9725805082	13.0691822026
N8	11.4670840921	10.2601465778	15.7118077663
N9	9.7170491962	9.3335109651	14.4727467175
N10	12.7911820861	7.3547326726	14.4025744118
C11	11.9200533694	10.4235558761	9.8337959104
C12	8.9550340622	12.4757219840	11.6154385765
C13	10.4519160093	15.7733771681	13.6182576073
H14	9.7685435388	16.5212399848	13.9985619995

C15	11.9094982929	14.6366862410	12.2384047687
H16	12.5217982649	14.3700319915	11.3894493174
C17	8.7158155267	14.6120644742	10.6992419223
H18	8.8444524470	15.4783486434	10.0640666810
C19	7.9041903906	14.5475555209	11.8732129918
H20	7.3087053112	15.3556057283	12.2774062610
C21	10.7487305924	14.5200227420	14.2245501590
H22	10.3433894925	14.1570419356	15.1580226640
C23	9.3785119436	13.3579756718	10.5539820781
H24	10.0898778891	13.0936573301	9.7848324108
C25	11.6888628377	13.7997218743	13.3946072747
C26	8.0606763693	13.2520589497	12.4434914456
H27	7.5895609091	12.8916505647	13.3470792680
C28	11.1750924735	15.8490438943	12.3896860891
H29	11.1305876313	16.6609911358	11.6760795755
C30	8.8691556545	8.2756764892	11.0849869536
H31	9.6669213499	8.1903868213	11.8268868433
H32	9.3106877274	8.0588573328	10.1053003106
H33	8.1312317840	7.4902549616	11.2833345644
C34	6.4841973336	10.0287497952	12.1611266087
H35	6.6858268837	10.0428900094	13.2360996378
H36	5.8405850847	9.1655069557	11.9536428094
H37	5.9002532299	10.9298724066	11.9458282929
N38	12.2197029549	11.0609793013	11.0197365740
N39	13.8985151911	11.3549704764	9.6055040901
H40	10.9859254384	9.9051919385	9.7019697361
C41	12.9488063704	10.5949178941	8.9456952596
H42	13.0858519906	10.2692200356	7.9257191701
C43	13.1014899163	8.2874851603	12.4285906200
C44	13.5449842923	7.2797463584	13.2390742930
H45	13.4267961523	8.5577029597	11.4358160392
C46	10.3976070384	11.0921889629	15.7091866125
C47	10.9518711925	8.9912466739	15.2324790977
H48	10.7155350371	8.2773840411	16.0605265146
C49	7.4608129030	10.3531828652	9.2913234827
C50	11.9267922265	8.3886085711	14.2526087392
C51	8.7383099217	8.2529111826	14.4468598197
H52	7.8577933886	8.5375083901	13.8749817241
H53	8.4272340323	7.9842743218	15.4700340848
H54	9.1789355608	7.3714774380	13.9715725854
C55	12.9602409795	6.4906096032	15.5637667760
H56	12.2672206792	6.7956822140	16.3467876287
H57	13.9811822791	6.5750322358	15.9463023257
H58	12.7603972992	5.4493708743	15.2947509269
C59	9.3152256664	10.6231604732	15.0015634959
H60	10.4764704872	12.0790581892	16.1489085778
H61	8.3189438928	11.0053843209	14.8549778713
H62	14.3090164481	6.5287774160	13.1084426402
C63	15.1649360361	11.8235544608	9.0635344005
H64	15.6802615508	12.4104365899	9.8254141993
H65	14.9966375316	12.4549110285	8.1862420297
H66	15.7987330249	10.9785602270	8.7785853250
C67	13.4131596038	11.6058401670	10.8488484135
H68	13.9353497744	12.1836369271	11.5941423613
X69	11.1016443261	10.7902596500	15.5508649012
X70	11.2548302868	14.9810507998	13.0087879514

X71	8.5059206104	13.6230131024	11.5767748329
C72	13.1749706904	12.9348129623	16.5868137914
H73	12.4746410699	13.7730693918	16.6759381485
H74	12.6971528347	12.0345066243	16.9820795685
H75	14.0398358786	13.1660682186	17.2191518596
C76	14.6181080373	10.9843724636	14.6795371908
H77	13.9393212022	10.1791582487	14.9651785893
H78	15.0110550289	10.7744576308	13.6781502711
H79	15.4616212845	10.9786374169	15.3784565697
C80	14.9810497281	14.0412323808	14.3670410849
C81	15.4391389741	14.0207315739	12.8944512843
H82	14.6201098630	14.2606612266	12.2102023884
H83	16.2310328650	14.7660567125	12.7237762783
H84	15.8568963776	13.0442670782	12.6131103923
C85	14.4321224337	15.4476440702	14.6960059300
H86	13.5613880437	15.7080864568	14.0894929339
H87	14.1427580682	15.5313286840	15.7492949104
H88	15.2037273066	16.2111441148	14.5119474392
C89	16.2393568019	13.8166695188	15.2405623448
H90	16.9612557253	14.6308493914	15.0768076090
H91	16.0082771636	13.8051334783	16.3112791995
H92	16.7503364736	12.8780144856	15.0002168778
C93	6.6047289211	11.6338952773	9.1747796551
H94	5.7191561422	11.5968566852	9.8179754738
H95	7.1667425243	12.5347825131	9.4316026450
H96	6.2444070307	11.7518214500	8.1417344587
C97	8.6242565673	10.4565879988	8.2848973010
H98	9.2882120443	11.2959814331	8.5100130941
H99	9.2300594328	9.5419853791	8.2594756116
H100	8.2363090704	10.6070945286	7.2664282712
C101	6.5738425605	9.1551472245	8.8714123422
H102	6.1982342067	9.3034326092	7.8481528316
H103	7.1215540903	8.2059782377	8.8803447176
H104	5.6984990302	9.0417741342	9.5207632220

TS 3^{Sc} to I$_{Sc}^{3-4}$

Sc	10.7763213633	11.1513096227	13.5051286382
N	12.2608694214	12.5933877937	13.5254276026
N	9.3095445177	11.1120640349	11.9906883677
Fe	9.6731532571	14.2057378691	12.6747971225
Si	8.4935180265	9.9416125510	10.9608034228
Si	13.8997098591	12.5801581773	14.1911993971
N	11.8083409694	9.1274132504	13.1472828199
N	11.5690266607	10.3176238125	15.7307119083
N	9.5603729025	9.5074271142	14.9264790290
N	12.3008552514	7.2398027329	14.1890729816
C	8.7831334354	12.4235754225	11.9704543844
C	10.3747326404	15.7687073020	13.8321689192
H	9.7411088567	16.4879310157	14.3335437572
C	11.6100275405	14.6849619055	12.2063305963
H	12.0721000970	14.4374949855	11.2618826163
C	8.1824190644	14.5833345935	11.3100060141
H	8.1170344987	15.5029087431	10.7438977284
C	7.6043444281	14.3470527698	12.5936882714
H	7.0171890518	15.0521389440	13.1666224253

C	10.8317556117	14.5318970446	14.3714788548
H	10.6298167430	14.1616929119	15.3661880153
C	8.9228880315	13.4214513157	10.9387866336
H	9.5205391353	13.3096093209	10.0471327830
C	11.6205528613	13.8397136194	13.3739174299
C	7.9690485493	13.0319405980	12.9995194104
H	7.6785363093	12.5467321611	13.9197641746
C	10.8663400458	15.8682327792	12.4948388594
H	10.6633039580	16.6742745867	11.8026196014
C	9.1887529072	8.2075670919	11.2932199480
H	9.2954088112	8.0140954436	12.3614469943
H	10.1707721407	8.0538071447	10.8359435891
H	8.5096168967	7.4536777631	10.8801309477
C	6.6356962667	9.9144377070	11.3757071832
H	6.4659513548	9.5188395531	12.3844036492
H	6.0666853382	9.2891330898	10.6782534533
H	6.2069555389	10.9216857566	11.3453036332
C	12.5979134591	8.3695355217	12.3175353269
C	12.9130181935	7.1947861964	12.9447525119
H	12.8883143601	8.7105548723	11.3355255869
C	10.5655530613	11.1862807128	16.0408891990
C	10.8942630290	9.0621609008	15.4093242970
H	10.7966330178	8.3747916223	16.2837198331
C	8.6457244419	10.2176825816	9.0337977671
C	11.6442785041	8.4236303206	14.2657715078
C	8.4727138511	8.5405394849	14.9375756400
H	7.5910865810	8.9651124204	14.4526347309
H	8.2107238028	8.2426128535	15.9655450864
H	8.7653419658	7.6485820709	14.3785997838
C	12.3907366381	6.1929788012	15.2012263725
H	11.9518119152	6.5470306639	16.1327861136
H	13.4394345793	5.9443983363	15.3807337407
H	11.8587615056	5.2956653798	14.8722660953
C	9.3408516914	10.7797937110	15.5674348697
H	10.7871569868	12.1442974828	16.4957324540
H	8.3513027683	11.2006087729	15.6499380776
H	13.5041328404	6.3470298039	12.6355977686
C	14.5767373588	10.8138057609	14.1556909977
H	14.6446994352	10.4045146042	13.1428069836
H	15.5797663225	10.7881280887	14.5947745892
H	13.9298621960	10.1686242946	14.7533400612
C	13.8764460757	13.1557526567	16.0018104555
H	13.3486551135	12.4099026905	16.6061477013
H	14.8863242602	13.2631545486	16.4144500119
H	13.3684161798	14.1187919078	16.1208814727
C	15.1543461762	13.7046740872	13.2096430708
C	16.5868552861	13.4163894009	13.7165393218
H	16.6930838184	13.6026275559	14.7915150005
H	16.8938417809	12.3831394469	13.5243079714
H	17.3067468496	14.0707562069	13.2037383197
C	15.1128387241	13.3873561656	11.7003141617
H	15.3563124205	12.3373534224	11.4986704108
H	14.1310465720	13.5854467079	11.2624283640
H	15.8476968929	14.0000490963	11.1574886751
C	14.8777348145	15.2090405689	13.4234753083
H	15.6146036449	15.8129944878	12.8730264760

H	13.8851257929	15.5050748808	13.0746707326
H	14.9569409281	15.4894128157	14.4800070936
C	7.6591951483	11.2845051898	8.5093366859
H	6.6189567134	10.9939063565	8.6896000403
H	7.8091910978	12.2644430437	8.9675460754
H	7.7761424898	11.4057518147	7.4228792317
C	8.2979854053	8.8906789273	8.3164233275
H	7.2975171007	8.5263411284	8.5777097044
H	8.3098398023	9.0395973968	7.2274505156
H	9.0127419441	8.0931333147	8.5420043262
C	10.0837267919	10.6084737789	8.6376819541
H	10.1686993908	10.7074598582	7.5459979668
H	10.3969563895	11.5579103622	9.0806945308
H	10.8117879809	9.8499535208	8.9501621536

I_{Sc}^{3-4}-imidazole

Sc	11.1131585753	10.9710964204	12.9446722374
N	12.4449840329	12.6050593692	13.3128901080
N	9.3953866599	11.2518429983	11.7589806412
Fe	9.8015182648	14.3047764257	12.6267406523
Si	8.3966295761	10.1349846796	10.8415572434
Si	13.9496604801	12.6433938455	14.2187935218
N	12.0314021423	8.8661089306	13.4297713585
N	10.8725235387	9.1761659418	16.5234078696
N	9.6265546736	9.6767083173	14.5236128480
N	12.2403659570	7.0476371129	14.6743002118
C	12.5980166904	9.4883671516	10.0740603129
C	8.9146436219	12.5796290363	11.8026470692
C	10.4610941573	15.6559489520	14.0533921613
H	9.8058690048	16.2828006345	14.6438040706
C	11.7557608389	14.8547191524	12.3213877696
H	12.2600770970	14.7765148672	11.3685660641
C	8.3818232739	14.7765258368	11.2086184634
H	8.3546056578	15.7195569748	10.6794017716
C	7.7450564192	14.4962578417	12.4544373187
H	7.1483721976	15.1885979426	13.0335580328
C	10.9032875966	14.3455433360	14.3971548892
H	10.6569807315	13.8083166083	15.3008139973
C	9.1108398510	13.6144674410	10.8174499902
H	9.7288027314	13.5192730782	9.9367126686
C	11.7365506013	13.8293277047	13.3369179326
C	8.0735139758	13.1593118988	12.8221220742
H	7.7531120945	12.6545509127	13.7226415705
C	10.9944877438	15.9761462091	12.7691988285
H	10.8144726151	16.8872733236	12.2139390889
C	9.1073390609	8.3884601471	11.0829645864
H	9.4531838915	8.2546392604	12.1124306504
H	9.9488089840	8.1813943837	10.4139125379
H	8.3393418085	7.6328609374	10.8816005108
C	6.5924758558	10.1352888100	11.4587983887
H	6.4905359305	9.6240846952	12.4203981202
H	5.9294179296	9.6268063850	10.7488421459
H	6.2157957667	11.1561457793	11.5841517575
N	12.4644132425	10.5340598166	10.9674990435
N	13.6754355856	11.2105718038	9.2394813844

H	12.1528873638	8.5236338452	10.2607761449
C	13.3481791107	9.8890593280	9.0009732183
H	13.6638636226	9.3743803462	8.1063075496
C	13.1401332896	8.1543602920	13.0008701325
C	13.2780088984	7.0266137317	13.7577964959
H	13.7648134779	8.5099887238	12.1991356302
C	10.7989949680	10.4665677533	16.3401607312
C	10.3436166325	8.6108871687	15.2686215862
H	9.6775445729	7.7589500482	15.4612343706
C	8.2660909912	10.4697126147	8.9193689600
C	11.5135667991	8.1656333548	14.4361298033
C	8.1731311217	9.5904767619	14.7146399078
H	7.6978046021	10.4098634763	14.1759149841
H	7.8939144413	9.6507217765	15.7780390278
H	7.7960925877	8.6495621385	14.2992730273
C	11.9863754658	6.0783866231	15.7342055714
H	11.7095510557	6.6144144421	16.6443478955
H	12.8987343276	5.5084493425	15.9167970617
H	11.1855723296	5.3868077353	15.4522135927
C	10.2207968808	10.9126753599	15.1006757265
H	11.1805018183	11.1416851923	17.1046522362
H	9.5395958150	11.7636649958	15.1241482325
H	14.0035704626	6.2282525671	13.7376987504
C	14.4448876295	12.0870964469	8.3689529218
H	14.6187917644	13.0326227218	8.8847851752
H	13.9012852842	12.2826142660	7.4399815080
H	15.4111975859	11.6341589326	8.1314104203
C	13.1222397716	11.5501258060	10.4304133590
H	13.2282518088	12.5158409503	10.8989311590
C	14.8188799818	10.9715339525	14.0211001483
H	15.0692103565	10.7472041303	12.9782058744
H	15.7488866204	10.9567108661	14.5992534275
H	14.1916258561	10.1589414962	14.3956789657
C	15.2108601309	14.0293142587	13.6566593027
C	13.6757006368	12.9068354336	16.0843317817
H	14.6211807419	13.0603094252	16.6181061626
H	13.0386502039	13.7739385766	16.2860344640
H	13.1923762675	12.0274953280	16.5215430875
C	16.5938658739	13.7254438770	14.2796439179
H	16.5477472900	13.6401139714	15.3714124390
H	17.0291768300	12.7983442826	13.8913984531
H	17.2987372309	14.5381502415	14.0503477441
C	14.7742177588	15.4287162403	14.1459066819
H	14.7019882919	15.4702066620	15.2382825149
H	15.5127324948	16.1861183375	13.8423105222
H	13.8062831891	15.7300386333	13.7372302104
C	15.3830786467	14.0670463763	12.1243909264
H	16.1648781078	14.7872127540	11.8392356769
H	15.6807498315	13.0900663048	11.7218065740
H	14.4602919401	14.3771025177	11.6238767805
C	9.6342047632	10.8002920571	8.2923135145
H	10.3540796324	9.9857718051	8.4257253548
H	9.5291844671	10.9705614432	7.2099663913
H	10.0783439771	11.7002945327	8.7278282037
C	7.2799339368	11.6168602649	8.6022783489
H	7.5881936183	12.5682790893	9.0434728678

H	7.2093643919	11.7642301206	7.5140249619
H	6.2690406099	11.3980526359	8.9630330886
C	7.7253556137	9.1901933415	8.2378414372
H	7.5900265057	9.3640790317	7.1601259755
H	8.4093153786	8.3415348660	8.3470077435
H	6.7506055844	8.8857839085	8.6371513797

I_{Sc}^{3-4}

Sc	10.6411762584	11.1896638324	13.3824295501
N	12.2057016898	12.5291541191	13.6918020532
N	9.2032160637	11.2863475217	11.8832591487
Fe	9.6319995713	14.2846708157	12.8333160572
Si	8.5115568578	10.1412732654	10.7536214610
Si	13.8148958453	12.5719305714	14.3992041938
N	11.8712019141	9.3004177541	13.1799323683
N	11.2322155318	9.2912212006	16.4762835542
N	9.6180789843	9.5918488797	14.7243067312
N	12.6628371174	7.5113568683	14.2051067937
C	8.6983821966	12.6006182401	11.9427336257
C	10.3529098672	15.7017651141	14.1668903564
H	9.7249108573	16.4004584139	14.7038604037
C	11.6222886208	14.7227729256	12.5040614804
H	12.1252591350	14.5429271013	11.5642002179
C	8.1963951637	14.8290675149	11.4595251332
H	8.1761441364	15.7946537099	10.9726003286
C	7.5709276433	14.5040013244	12.7003630619
H	6.9890727268	15.1777072545	13.3152221211
C	10.7351809087	14.4042680311	14.6085919592
H	10.4753764348	13.9427981160	15.5505671596
C	8.9081374444	13.6787393545	11.0079776839
H	9.5276655782	13.6243860641	10.1253626548
C	11.5590033809	13.7819765816	13.5949870682
C	7.8769274049	13.1453750911	12.9993134144
H	7.5490290962	12.5938285436	13.8703123149
C	10.9073247742	15.9022849103	12.8656143974
H	10.7705214667	16.7785695194	12.2456185120
C	9.2588517668	8.4317723160	11.1100972438
H	9.2405516808	8.1998463549	12.1774600232
H	10.2999117176	8.3554362382	10.7787332281
H	8.6879198770	7.6556748444	10.5882355843
C	6.6283460202	10.0457427042	10.9999069428
H	6.3861175874	9.6204246749	11.9809751622
H	6.1419541327	9.4214162547	10.2412315968
H	6.1724930269	11.0407882145	10.9532292014
C	12.9507936905	8.8277708829	12.4618893902
C	13.4484991250	7.7162294372	13.0825404956
H	13.2966347908	9.3217817048	11.5669404968
C	10.7124139607	10.4853857213	16.5341612669
C	10.6553083852	8.6662138801	15.2809116475
H	10.2150703087	7.6876929583	15.5288466107
C	8.8565847102	10.5160185701	8.8751590663
C	11.7172719768	8.4799300638	14.2197852397
C	8.2573159030	9.0437190507	14.7133145721
H	7.5857677478	9.7656849782	14.2442294096
H	7.9012910914	8.8298341031	15.7320501152

H	8.2257664872	8.1237342762	14.1232019415
C	12.8377247373	6.4711851028	15.2141135476
H	12.6246847913	6.8925816745	16.1981811183
H	13.8735866298	6.1292770009	15.1923088187
H	12.1766242986	5.6204121606	15.0210403940
C	9.7850658197	10.8498014233	15.4963788287
H	11.0140023958	11.1643436172	17.3303666048
H	8.8615046084	11.3629518789	15.7608290766
H	14.2762679495	7.0666832645	12.8439922858
C	14.2973024711	10.8624452758	15.0619874127
H	14.5077160020	10.1396746500	14.2678691163
H	15.2064300136	10.9567885288	15.6676926005
H	13.5163515100	10.4438901162	15.7043377868
C	15.1916556233	13.1264890376	13.1380472399
C	13.8663315344	13.7682005426	15.8774647286
H	14.8799437930	13.8388847008	16.2904180424
H	13.5449922883	14.7795567871	15.6098424782
H	13.2093516906	13.4158825006	16.6811004404
C	16.5827230349	12.7278644989	13.6819844433
H	16.7854568634	13.1724350645	14.6641309889
H	16.6942972719	11.6428088004	13.7796225439
H	17.3727574849	13.0785040764	13.0018900251
C	15.1907903345	14.6569325173	12.9304885197
H	15.4019210658	15.1933515556	13.8624578969
H	15.9691216892	14.9441591731	12.2078859691
H	14.2356602347	15.0272978719	12.5480430359
C	14.9795626135	12.4360698840	11.7752078257
H	15.7648569093	12.7305093516	11.0630039166
H	15.0164981320	11.3426770909	11.8641450767
H	14.0117066519	12.6972746438	11.3347258396
C	10.3215834486	10.9561365458	8.6710528239
H	11.0278011144	10.1912659720	9.0179569397
H	10.5295474307	11.1292833838	7.6049325129
H	10.5558979929	11.8795318078	9.2092485464
C	7.9089366506	11.6006057698	8.3168961033
H	7.9922704352	12.5508200536	8.8504921639
H	8.1354538511	11.7957559188	7.2584039460
H	6.8605985335	11.2857938228	8.3698026730
C	8.6198479951	9.2263972874	8.0547382823
H	8.7478765347	9.4309411478	6.9819955022
H	9.3236399995	8.4309247984	8.3206728383
H	7.6049097686	8.8318421702	8.1868149117

TS $I_{Sc}^{3\text{-}4}$-imidazole to 4^{Sc}-imidazole

Sc	11.2079364597	11.6185795777	12.1988999233
N	10.5931609206	13.4985033741	13.0878174140
N	10.1032208610	9.8290888115	12.4016769207
Fe	9.0726760845	11.4044892528	15.0108080695
Si	10.0286756662	8.3242657612	11.4969326371
Si	11.1576149289	15.1597180374	12.9410031773
N	12.7719849950	12.1797993246	10.5959961502
N	14.8458203835	12.4300906763	13.1019149957
N	13.1366057512	10.4601547933	12.7118577231
N	14.7456728739	12.1626105281	9.5740956651
C	9.4299672780	11.6706682896	9.1431929871

C	9.3845946715	9.8424558081	13.6178598134
C	9.4379523184	12.7540274390	16.5386127426
H	9.5607720452	12.4749421093	17.5769871325
C	8.4794656754	13.2996557620	14.5128577419
H	7.7423282186	13.5118663052	13.7516740963
C	7.6446471220	9.9346580128	15.1781263492
H	6.6725856017	10.0977002522	15.6246478445
C	8.8291764823	9.5371278480	15.8698324204
H	8.9102641305	9.3440181680	16.9314121815
C	10.4756336777	12.8496531516	15.5672260219
H	11.5253267517	12.6737122572	15.7456344831
C	7.9856974103	10.1434873737	13.8082289311
H	7.3170388690	10.4803588242	13.0292520044
C	9.9050567528	13.2181582375	14.2911409064
C	9.8928227454	9.4888030418	14.9235552570
H	10.9203507300	9.2299341968	15.1351184824
C	8.2001097293	13.0429124880	15.8892621170
H	7.2199739588	13.0207719320	16.3471122644
C	11.1682511891	8.5175342550	9.9803126607
H	11.9491249823	9.2677799638	10.1518641947
H	10.6180016781	8.8038980213	9.0772890149
H	11.6671888181	7.5672137054	9.7559111698
C	10.6319850703	6.8388793076	12.5305270763
H	11.7223431918	6.8000961309	12.5936926082
H	10.2978138745	5.8903661773	12.0955279713
H	10.2427085449	6.8840648663	13.5530553478
N	9.7173680247	12.1944113574	10.3886459107
N	7.9479551718	13.2383635682	9.5528858312
H	10.0207794321	10.8776143593	8.7136581623
C	8.3418575677	12.3085759711	8.6094052778
H	7.8183852943	12.1813515194	7.6747081875
C	12.6031927592	12.5362848039	9.2710084792
C	13.8049828061	12.5136938401	8.6257906450
H	11.6358868062	12.7887721773	8.8743535936
C	13.8241693400	12.3396408973	13.9410351982
C	14.8287943976	11.6655456299	11.9883104723
H	15.8126448477	11.2425109134	11.7489346455
C	8.2634955847	7.7775110844	10.8577805637
C	14.0890335705	11.9744334275	10.7667651045
C	13.3527342198	9.0267613842	12.9159967452
H	12.5730506461	8.5917924605	13.5508486078
H	14.3232325951	8.8401433421	13.3975528372
H	13.3390263557	8.5036517380	11.9560571607
C	16.1793422734	12.0631964316	9.3276884102
H	16.7348927380	12.6401732237	10.0715496799
H	16.3880481597	12.4716073320	8.3360298963
H	16.5180829147	11.0218230303	9.3550819355
C	13.0079943123	11.1916738514	13.8700818907
H	13.7800953620	13.0214415523	14.7843981686
H	12.7076896152	10.7233506884	14.8098524451
H	14.0772335811	12.7159951871	7.6012939057
C	6.8181194080	14.1528465868	9.4613849195
H	6.8447552806	14.8309694730	10.3150189049
H	5.8729086980	13.6014751186	9.4717859008
H	6.8799084264	14.7419013456	8.5422582414
C	8.8022953263	13.1288754088	10.6002287865

H	8.7668563700	13.7439945264	11.4836085332
C	11.8329767652	15.4129262515	11.1883952231
H	11.0716708385	15.2554797948	10.4158811528
H	12.2257400491	16.4290865901	11.0717323301
H	12.6514050149	14.7171405250	10.9879991355
C	9.7945402311	16.5393886641	13.2345710322
C	12.5609808979	15.5803587221	14.1573487990
H	12.7316390399	16.6615635118	14.2115518030
H	12.3425538414	15.2323403532	15.1733941100
H	13.5009004602	15.1182609493	13.8379068171
C	10.3652157008	17.9060675924	12.7796616264
H	11.2980710971	18.1631887563	13.2946262303
H	10.5614297930	17.9349648505	11.7020938109
H	9.6432786552	18.7069466873	13.0015867366
C	9.4184556715	16.6637669881	14.7286377212
H	10.2852868104	16.9308938776	15.3421171168
H	8.6684870566	17.4574337110	14.8676186224
H	8.9979940649	15.7379500701	15.1319667905
C	8.5069204991	16.2874154350	12.4217524489
H	7.8042723413	17.1268184431	12.5398855208
H	8.7151800623	16.1932417713	11.3486182264
H	7.9842577438	15.3860394497	12.7556375968
C	7.4946268679	8.9380001534	10.1987801619
H	8.0068178098	9.3139262081	9.3079304852
H	6.4961540141	8.6043780675	9.8810846205
H	7.3615721503	9.7856854480	10.8766396313
C	7.4021637443	7.1951766255	12.0012396960
H	7.2142782845	7.9231748603	12.7949046039
H	6.4260527761	6.8728809494	11.6095811688
H	7.8702144990	6.3174034553	12.4592639962
C	8.4456270408	6.6639626466	9.7981535324
H	7.4640189910	6.3120008835	9.4483225597
H	8.9963233856	7.0118800470	8.9175038933
H	8.9735258662	5.7899620171	10.1962164968

TS I_{Sc}^{3-4} to 4^{Sc}

Sc	10.5855085158	11.2599274194	13.4612835295
N	12.2055847601	12.5602565176	13.7449356008
N	9.3160454728	11.2543894910	11.8122067324
Fe	9.6643320855	14.2506449192	12.7759243058
Si	8.5950322170	10.0655452805	10.7410647679
Si	13.8306891409	12.5735455262	14.4210863899
N	11.8022756856	9.4168495398	13.3878652054
N	11.3060890053	9.5099110158	16.6151419248
N	9.4464646177	9.8850400216	14.7999446632
N	12.4442231725	7.4001284562	14.0235800064
C	8.7963190305	12.5619709572	11.8423094665
C	10.2838004158	15.7002038091	14.1198144014
H	9.6131247379	16.3841244172	14.6223738904
C	11.6460777178	14.7426875991	12.5178258422
H	12.1889618014	14.5699923697	11.5997627215
C	8.2882889021	14.7834794336	11.3412328385
H	8.2806148244	15.7511035702	10.8579259045
C	7.6139857569	14.4508675976	12.5551290895
H	7.0007366450	15.1182746001	13.1452845967

C	10.6878372404	14.4201425111	14.5916451390
H	10.4125890807	13.9690590352	15.5346280995
C	9.0316409374	13.6422349534	10.9175893570
H	9.6868733560	13.5905304922	10.0606722009
C	11.5659860502	13.8085927042	13.6144970568
C	7.9224185961	13.0953545850	12.8659807129
H	7.5532111049	12.5350066808	13.7148036385
C	10.8843064286	15.9040947529	12.8400267463
H	10.7428840301	16.7678043896	12.2041780585
C	9.3135726258	8.3640771273	11.1743324162
H	9.3164261265	8.1947157267	12.2547739946
H	10.3423142333	8.2388830962	10.8227036458
H	8.7092202608	7.5752927488	10.7127258575
C	6.7130816000	10.0041840136	11.0032411930
H	6.4728874941	9.6138299840	11.9982624976
H	6.2191442597	9.3592995361	10.2674232863
H	6.2637849433	10.9998002255	10.9248922494
C	12.6258180182	8.8921289315	12.4170256106
C	13.0230272421	7.6401443990	12.7914217364
H	12.8677476099	9.4419154755	11.5203724962
C	10.8026310027	10.7292611128	16.5239430873
C	11.0160088970	8.6034268027	15.6566815368
H	10.8162035146	7.6049518868	16.0644726903
C	8.9198831988	10.3647741125	8.8458657093
C	11.7065654490	8.5039463615	14.3637113194
C	8.0621737943	9.4165547631	14.7071316103
H	7.3841143008	10.2243169347	14.3993642831
H	7.7034892501	9.0268229723	15.6697099295
H	7.9883964569	8.6215618784	13.9616005804
C	12.6541765976	6.1979582534	14.8241309711
H	12.9286623436	6.4663313935	15.8460907469
H	13.4693301603	5.6257002911	14.3791700774
H	11.7568625132	5.5723991802	14.8441395247
C	9.6729708462	10.9164208929	15.6927055967
H	11.1224131967	11.4849384648	17.2353461638
H	8.8568760031	11.5344224908	16.0752321656
H	13.6514866305	6.9094378564	12.3069149500
C	14.3567020241	10.8218829908	14.9165806621
H	14.4994197949	10.1576131706	14.0590157300
H	15.3076489422	10.8732663325	15.4584783716
H	13.6232496573	10.3637231172	15.5863741865
C	15.1806724395	13.2661677715	13.1984439138
C	13.8711849531	13.6257989711	16.0047410873
H	14.8906901187	13.7327644540	16.3926993392
H	13.4697302166	14.6313274077	15.8444869748
H	13.2699536003	13.1526664749	16.7902921818
C	16.5860797369	12.8423142894	13.6843914201
H	16.7925701139	13.1843266939	14.7056378435
H	16.7219767418	11.7560605940	13.6634549893
H	17.3590884731	13.2802505272	13.0362382643
C	15.1552739851	14.8094441417	13.1348355932
H	15.3818309570	15.2595436931	14.1077122122
H	15.9135767285	15.1733416812	12.4256007174
H	14.1875670326	15.2005774154	12.8090845211
C	14.9677508439	12.7011316485	11.7790147983
H	15.7391519469	13.0777949524	11.0915774060

H	15.0292126793	11.6057660105	11.7641813812
H	13.9911777209	12.9782977884	11.3702791898
C	10.3901635732	10.7564805319	8.5957246224
H	11.0837390761	9.9831666338	8.9486877724
H	10.5765227274	10.8908826224	7.5206253332
H	10.6599152316	11.6900808279	9.0989989732
C	7.9979170762	11.4643984869	8.2748586264
H	8.1270062451	12.4254803685	8.7801988570
H	8.2102417263	11.6215606955	7.2073470898
H	6.9406662602	11.1896014464	8.3559959375
C	8.6258996896	9.0587760990	8.0709613767
H	8.7441272105	9.2251028934	6.9907427709
H	9.3061961932	8.2475791709	8.3502753042
H	7.6006605486	8.7038591093	8.2295801677

4^{Sc}

Sc	4.0920910663	10.6982531096	4.0005307020
Fe	2.8647324048	7.6639504104	5.1755680124
Si	4.8735098847	9.0302085277	1.0689069479
Si	3.6094952155	11.8656258056	7.2971380248
N	6.2290463207	11.3575209861	4.2181782098
N	2.0756845373	11.3240512049	3.0772965582
C	2.9061305771	9.4593139122	6.3020485259
N	4.2975518937	12.8746511418	3.1324960292
C	3.4814703242	8.3533242868	7.0252314050
H	4.5022149692	8.3160803809	7.3787206420
C	2.5463734691	7.3850463364	3.1331015133
H	1.7802943559	7.8598862319	2.5371017341
C	5.5269729600	13.4026488328	3.2240716655
H	5.7546645268	14.4056078113	2.8672991220
N	0.8117933155	12.8872578438	2.1259154374
C	2.0523340803	12.5852841629	2.6114223421
C	7.2831893891	10.5473246163	4.8037753285
H	8.2511248180	11.0679497968	4.8113711705
H	7.3971078638	9.6113023107	4.2442326859
H	7.0274694115	10.2817021094	5.8376654685
C	0.8150508659	10.8095704069	2.8690365476
H	0.5650435492	9.7981248592	3.1494790867
C	6.5125132383	12.5677600509	3.7903423827
H	7.5358924590	12.9501627374	3.8753858214
C	0.0206208808	11.7571721911	2.2851214147
H	-1.0115204665	11.7404917729	1.9716609469
C	3.2110043949	13.4269415053	2.6284984454
H	3.1977566626	14.4380981650	2.2220148455
C	2.1284179298	13.9844106785	8.5305845795
H	1.1670857269	14.4749618337	8.7434393282
H	2.7858857490	14.7380544465	8.0835814655
H	2.5607453124	13.6951264713	9.4960432354
C	3.8770041927	7.9097466777	3.3282405418
C	5.6336257837	10.7085768166	0.6246301419
H	4.9469122424	11.5321743940	0.8457827487
H	5.8581631381	10.7513855380	-0.4471230198
H	6.5629237668	10.8995297979	1.1705102266
C	2.4283529291	6.1483452555	3.8301461460
H	1.5430083947	5.5291927164	3.8852020427

C	4.9220142545	13.1690243022	6.8878379356
H	5.8989316381	12.6935244193	6.7558099415
H	5.0097080554	13.8830568234	7.7145843765
H	4.7072749315	13.7362523988	5.9770225489
C	1.5528303403	9.0685759283	5.9865110490
H	0.8490870461	9.6791131919	5.4403178552
C	6.1537900174	7.6311263221	0.6569128392
C	3.3470953986	8.7813238493	-0.0382652817
H	2.6307619813	9.5954922774	0.1213767742
H	2.8318635122	7.8402786224	0.1805927741
H	3.6115538205	8.7732415830	-1.1024468140
C	4.5512238610	6.9767522257	4.1962505018
H	5.5602699888	7.0970220302	4.5646966103
C	7.3310620835	7.6660910854	1.6532539403
H	8.0738656098	6.8952574631	1.4002457262
H	6.9975646090	7.4791794130	2.6783341045
H	7.8493923974	8.6327048879	1.6418284085
C	5.4969303012	6.2331595110	0.7068418161
H	6.2380606539	5.4569996104	0.4642986083
H	4.6825157711	6.1388972841	-0.0205103506
H	5.0903812314	5.9999842407	1.6949869002
C	2.4951792509	7.3369378508	7.1823693502
H	2.6376527903	6.3798190050	7.6665436201
C	1.3027188250	7.7757356617	6.5320681933
H	0.3823151998	7.2131952391	6.4453607972
C	6.7113127475	7.8466780883	-0.7682359910
H	7.4077843032	7.0366758216	-1.0296659839
H	7.2612972815	8.7897989725	-0.8591886196
H	5.9196275101	7.8464448611	-1.5271056628
C	4.1297611976	11.0473416179	8.9330977898
H	5.1323891444	10.6129954215	8.8462375902
H	3.4490291647	10.2448617792	9.2333834107
H	4.1596422845	11.7807324779	9.7478305017
C	0.8888374365	11.8297320165	8.2681873866
H	-0.0659467482	12.3546090680	8.4228661108
H	1.2302418597	11.4856962302	9.2510661447
H	0.6813782483	10.9428059610	7.6621879590
C	1.9149216723	12.7704448404	7.5991609360
C	3.6699964066	5.8940651449	4.4872784680
H	3.8872599352	5.0503058233	5.1281916639
C	1.3305498068	13.2730712939	6.2628548881
H	0.3879614475	13.8151319569	6.4344349653
H	1.1202674936	12.4467739531	5.5768168719
H	2.0140267410	13.9616637240	5.7501722723
N	3.5344637862	10.6843640529	5.9963000751
N	4.4228140070	9.0776900722	2.7639423634
C	0.4046189883	14.1577475835	1.5506248506
H	0.9892013753	14.3832906454	0.6531448642
H	0.5324659012	14.9694100516	2.2735647598
H	-0.6490411179	14.0986121895	1.2748606705

6^{Sc}-py-py

Fe1	1.0147546812	0.8015274789	8.6214453852
Sc2	2.9645829272	2.4914971852	10.6965534516
Si3	2.1701841253	5.4469516736	8.9041107324

Si4	2.6964416006	-0.1351088460	13.0275697553
N5	2.3029225027	0.7436762116	11.5489905325
N6	2.1848460986	3.7155548316	9.2300367913
N7	5.0846981121	1.9917824220	10.0587022931
N8	4.1494962503	3.6277065358	11.9764856602
C9	6.7636848417	0.8756866798	8.7554622105
H10	7.0083711836	0.1353219874	8.0012887255
C11	2.0194381665	-0.7907058228	9.5393460170
H12	3.0567405903	-1.0698790002	9.4125364701
C13	3.7146993300	4.3397654400	13.0651996282
C14	5.8679131457	4.2202808612	14.1179676486
C15	5.4444953693	1.0883919184	9.1214349340
C16	1.5290084184	0.0970519691	10.5680396433
C17	6.0339469047	2.7218590705	10.6815893991
C18	2.6487794885	-2.0050463485	12.6975951173
H19	3.4168491692	-2.2915454258	11.9703830858
H20	1.6833207066	-2.3357996713	12.3021304881
H21	2.8436395639	-2.5683817268	13.6176986568
C22	7.7531625633	1.6424592412	9.3777967514
H23	8.7988402890	1.5131748728	9.1131311675
C24	1.4582945683	0.2755584885	14.4601397175
C25	4.4545445126	0.3042848329	13.5717677183
H26	5.1639848976	0.0556900933	12.7737576955
H27	4.7400167240	-0.2761857511	14.4568995625
H28	4.5841016035	1.3646211651	13.8060014086
C29	5.5972993224	3.7207611166	11.7353236303
H30	5.8088458540	4.7221218051	11.2919941874
C31	3.5776513588	5.9806087361	7.6799951687
C32	0.1039097352	0.1790858043	10.3797593770
H33	-0.5609930221	0.7969822725	10.9676755622
C34	7.3844668453	2.5721302607	10.3417054376
H35	8.1294050376	3.1837157171	10.8391998870
C36	0.0757390048	-0.3506385039	14.1796566885
H37	-0.6318626705	-0.0968676179	14.9826829548
H38	0.1239418460	-1.4441195827	14.1240873496
H39	-0.3543521257	0.0093121682	13.2390828404
C40	4.5261646726	4.7593047399	14.0831659763
H41	4.1151555485	5.3013504364	14.9270647089
C42	6.3847633638	3.6098913975	13.0317479753
C43	3.6319739409	7.5218264814	7.5829775735
H44	4.4086393647	7.8331195477	6.8690364734
H45	3.8716044383	7.9868007480	8.5457064519
H46	2.6846453928	7.9480984334	7.2328495303
C47	1.2481446783	1.2716867314	6.6152163841
H48	1.4396016959	0.5419527916	5.8397885053
C49	3.3207088651	5.4097316068	6.2688365880
H50	4.1250073302	5.7101373143	5.5808783509
H51	2.3789971537	5.7752903646	5.8439973859
H52	3.2802861574	4.3155756908	6.2683671556
C53	2.2306366594	1.9715605018	7.3740296699
H54	3.3022741912	1.9063336582	7.2468403032
C55	0.9180110499	-1.2663627478	8.7736863338
H56	0.9704243492	-1.9363414249	7.9257912914
C57	0.5022219247	5.9754188117	8.1637530072
H58	-0.3111667547	5.7866046366	8.8736279159
H59	0.2630104839	5.4417429845	7.2386984906

H60	0.4971180748	7.0487610244	7.9407107235
C61	1.5662988206	2.8443858945	8.3145833666
C62	-0.2684920941	-0.6680428484	9.2960510606
H63	-1.2693428530	-0.8024356251	8.9089099206
C64	2.3822439853	6.3862446801	10.5334887372
H65	1.6020929124	6.0939399677	11.2462476218
H66	2.2793668212	7.4645170043	10.3660184733
H67	3.3484186839	6.2110141020	11.0141727470
C68	4.9450904037	5.4714784192	8.1784198069
H69	5.7483541692	5.7903157919	7.4976261657
H70	4.9718398275	4.3782272946	8.2323735024
H71	5.1906441496	5.8620612171	9.1736532110
C72	-0.0365219870	1.6860146654	7.0791638761
H73	-0.9881304879	1.3149469609	6.7235721101
C74	0.1547759921	2.6232439029	8.1348968472
H75	-0.6209564823	3.1005127508	8.7171509467
C76	1.9935588038	-0.2939263271	15.7928944776
H77	1.2761892997	-0.1071196343	16.6050882838
H78	2.9429413678	0.1677208407	16.0847546498
H79	2.1498482769	-1.3784997977	15.7462240099
C80	1.2930286325	1.8022924570	14.6032008393
H81	0.6159680800	2.0420637170	15.4365500185
H82	0.8624553068	2.2425694575	13.6958769030
H83	2.2461716597	2.3069355543	14.8004058074
H84	4.6319198612	0.5317903542	8.6649285342
H85	7.3259590370	3.0697802119	13.0598948199
H86	6.4150306201	4.2222479513	15.0588358070
H87	2.6372469501	4.4946380644	13.1254779552

8^{Sc}

Fe1	0.5273717443	1.1135442825	8.7475208674
Sc2	3.0416410630	2.5266388546	10.6447598377
Si3	2.9943029545	5.1905265169	8.3648673693
Si4	2.8962727376	-0.3306051808	12.6417006821
N5	2.3281125301	0.7136150538	11.3574633132
N6	2.5812622243	3.5770525756	8.9166694048
N7	4.9444888403	1.4521741733	9.6636372771
N8	5.1013664901	3.3432395797	11.6342330381
C9	5.9849680440	-0.0727633609	8.1320621843
H10	5.8656033863	-0.8539063379	7.3891601234
C11	1.2492677252	-0.6841627691	9.5140084341
H12	2.1246117430	-1.2198943665	9.1737429390
C13	5.2085664097	4.2425399054	12.6760492634
C14	2.7315234144	4.6543974621	13.1553756232
C15	4.8615716704	0.4895276348	8.7410534700
C16	1.2395441085	0.2935910242	10.5761178855
C17	6.1660699001	1.8975215587	10.0359277277
C18	3.4908137688	-2.0024992274	11.9487075679
H19	4.3278451000	-1.8527803790	11.2560790836
H20	2.6975704210	-2.5214195307	11.4003981094
H21	3.8368859826	-2.6749026305	12.7427453193
C22	7.2465440146	0.3918987863	8.5019005261
H23	8.1428374408	-0.0199159871	8.0475613796
C24	1.5545846576	-0.6774532550	13.9980097903
C25	4.3923929368	0.5118673664	13.4478025829

H26	5.2170929865	0.6135915801	12.7341904716
H27	4.7629067577	-0.0899691524	14.2849258448
H28	4.1553962059	1.5089938643	13.8332720822
C29	6.1954586706	2.9044843652	11.0839797425
H30	7.1747390985	3.2575108583	11.4229534744
C31	3.7761159441	5.2017164573	6.5849908685
C32	-0.1244623856	0.7510441620	10.6838445015
H33	-0.4639759780	1.5126983994	11.3717249235
C34	7.3431094481	1.3893037062	9.4678558712
H35	8.3077865988	1.7708749493	9.7881027757
C36	0.4551553620	-1.6217411230	13.4610781478
H37	-0.3007580638	-1.8052828628	14.2390004760
H38	0.8605980906	-2.5975456772	13.1695338362
H39	-0.0636032580	-1.2036348778	12.5934289367
C40	4.1568531554	4.8010549789	13.3446062658
H41	4.4575419053	5.4774027859	14.1447316692
C42	2.1485997108	3.8810676814	12.1980622849
C43	4.3799278841	6.5950196668	6.2968671351
H44	4.7990981288	6.6269686624	5.2803825043
H45	5.1895880410	6.8471073757	6.9905621794
H46	3.6282410749	7.3909311892	6.3589625128
C47	0.4840779226	1.4698373554	6.7104630461
H48	0.2986629335	0.7045062812	5.9684158589
C49	2.7192840614	4.9046604555	5.4986001435
H50	3.1812948124	4.9264850113	4.5001173746
H51	1.9160450502	5.6501960702	5.4981544995
H52	2.2582643658	3.9208502921	5.6255396994
C53	1.7567410602	1.8427658253	7.2344357638
H54	2.7122878801	1.4419102773	6.9291188085
C55	-0.0775611611	-0.8477205484	9.0206344135
H56	-0.3825160571	-1.5017578481	8.2144070283
C57	1.4719383739	6.3285116391	8.3628742681
H58	1.0745779383	6.4235809365	9.3801309048
H59	0.6681167911	5.9413613831	7.7283538154
H60	1.7189354926	7.3361066248	8.0077911077
C61	1.5760630653	2.8887116711	8.2127764520
C62	-0.9278291850	0.0415237160	9.7441471415
H63	-1.9875185854	0.1811653805	9.5783118464
C64	4.2584709149	5.9258578000	9.5674969309
H65	3.8975261845	5.8553044050	10.5974639115
H66	4.4144139970	6.9872071681	9.3433677253
H67	5.2343636898	5.4313487003	9.5140998742
C68	4.9008851762	4.1491783427	6.4904641121
H69	5.3692404157	4.1705892216	5.4950710962
H70	4.5223071820	3.1360259365	6.6579131777
H71	5.6945784525	4.3303602487	7.2262729823
C72	-0.5073377404	2.2565473532	7.3702662340
H73	-1.5763335163	2.1829605246	7.2223555109
C74	0.1532915248	3.1087328787	8.3011204400
H75	-0.3174117007	3.8076864675	8.9785833372
C76	2.2099419722	-1.3533348726	15.2235670439
H77	1.4456515652	-1.5987981330	15.9752631963
H78	2.9450489529	-0.7029825058	15.7102974631
H79	2.7143302646	-2.2912387680	14.9610757370
C80	0.9025389211	0.6447184191	14.4547789309
H81	0.1615153780	0.4546899905	15.2453690893

H82	0.3882727602	1.1486158435	13.6312223535
H83	1.6394741065	1.3493052914	14.8579786130
H84	3.8579367169	0.1639992599	8.4872541398
H85	1.0502717353	3.9237168788	12.2375018613
H86	2.1381904156	5.2430278126	13.8621636370
H87	6.2228472771	4.5125766276	12.9762660744

9^{Sc}

Fe1	1.0604357953	0.7684645804	8.1963020163
Sc2	3.2065074709	2.1312868253	10.4620452892
Si3	2.1334360744	5.2078658752	9.1329920842
Si4	1.9893065956	-0.1655222432	12.7984837128
N5	2.1300141616	0.5256857794	11.1883377761
N6	2.4861025046	3.4879797763	9.0493323453
N7	5.1143638316	0.9791841757	9.8145035337
C8	6.5889836048	4.1393294246	9.9863024867
C9	6.4193077495	-1.0203534788	10.1092876980
H10	6.4363507200	-2.0870048043	10.3063471398
C11	1.6009140298	-0.9818576267	9.1969958479
H12	2.5522855486	-1.4872828341	9.1082268584
C13	7.1738182358	4.0794027036	11.3363529224
C14	5.1145642694	3.4563116440	12.7330781989
C15	5.2067819615	-0.3431830705	10.0626513989
C16	1.2806240002	0.0349182315	10.1715149199
C17	6.2498034043	1.6859689835	9.6045611722
C18	1.5544615291	-2.0107428595	12.6728114334
H19	2.3589811002	-2.5672781585	12.1778063042
H20	0.6385318680	-2.1776174642	12.0973896781
H21	1.4110272563	-2.4549280637	13.6649793846
C22	7.5928905867	-0.2945186653	9.9117827478
H23	8.5613504730	-0.7850888443	9.9495134226
C24	0.6514917616	0.7187881463	13.8942657714
C25	3.6741926721	-0.0312528720	13.6592674432
H26	4.4564552064	-0.4943446275	13.0465807640
H27	3.6592209345	-0.5514416286	14.6236441121
H28	3.9675549887	1.0069118202	13.8364058269
C29	6.1259192804	3.1199470970	9.2494564825
H30	5.6422602615	3.3361063629	8.2987348023
C31	2.5850016752	6.1361188157	7.4874119383
C32	-0.0742183360	0.4365903209	9.8971509846
H33	-0.6024329732	1.2223603063	10.4192055878
C34	7.5053936986	1.0707410633	9.6578601385
H35	8.3927266647	1.6693144372	9.4855806664
C36	-0.7663508903	0.1979866242	13.5719149047
H37	-1.5157927027	0.7315082127	14.1749461770
H38	-0.8708355677	-0.8695820379	13.7962621164
H39	-1.0328921137	0.3396483399	12.5198052464
C40	6.5508171964	3.7648308121	12.4913844919
H41	7.1362062009	3.8708033373	13.4054779910
N42	4.2620336229	3.0016003191	11.9186626974
C43	2.6051524080	7.6590631187	7.7500241155
H44	2.8311509812	8.2026149094	6.8211447310
H45	3.3647404499	7.9423660516	8.4866867989
H46	1.6376004820	8.0283991663	8.1106878983
C47	1.7876068377	1.1321788664	6.2903583948

H48	2.0468188278	0.3617767777	5.5765984473
C49	1.5638098013	5.8578332611	6.3623070501
H50	1.8420844149	6.4113582332	5.4532542399
H51	0.5530355400	6.1793742180	6.6381950953
H52	1.5149180220	4.7973570923	6.0991974945
C53	2.6689461371	1.7298110664	7.2407654793
H54	3.7214871481	1.5085561374	7.3576475955
C55	0.4625263994	-1.2119545306	8.3734199039
H56	0.4064227879	-1.9017474287	7.5417244892
C57	0.3112290442	5.5663476970	9.5599830484
H58	0.0225628547	5.0126131317	10.4613277780
H59	-0.3884270549	5.2919032860	8.7645176999
H60	0.1618481767	6.6326562289	9.7699981435
C61	1.9423883334	2.7068815837	8.0154787524
C62	-0.5758659372	-0.3340280369	8.8064806270
H63	-1.5566666606	-0.2416437518	8.3599754241
C64	3.1479318407	5.9438442771	10.5524525928
H65	2.9718419752	5.4005050250	11.4861424747
H66	2.8597441961	6.9882998925	10.7158264438
H67	4.2248513906	5.9172875957	10.3607514511
C68	3.9817523101	5.6987240406	6.9995737006
H69	4.2652776240	6.2510325493	6.0916479671
H70	4.0048807901	4.6306062799	6.7583893107
H71	4.7569006986	5.8927108050	7.7515325284
C72	0.5026227525	1.7264256563	6.4578336330
H73	-0.3906552999	1.4765345125	5.9015538526
C74	0.5827668205	2.6595279509	7.5348397179
H75	-0.2393136951	3.2339184853	7.9351590707
C76	0.9363635884	0.4400412337	15.3871396987
H77	0.1505165596	0.8846297509	16.0147147286
H78	1.8920860185	0.8666266521	15.7096063992
H79	0.9579080434	-0.6336533018	15.6119673332
C80	0.6893772978	2.2434134382	13.6613907613
H81	-0.0241653164	2.7534215237	14.3253989908
H82	0.4214807947	2.5008188441	12.6305504820
H83	1.6822754935	2.6666850968	13.8535636063
H84	4.2665426246	-0.8453395822	10.2550001644
H85	4.8272433091	3.7024791373	13.7775626031
H86	8.1984188394	4.4489689260	11.4137884059
X87	0.2717918204	-0.0891448831	9.9077504752
X88	0.6925671665	2.3133190167	7.5658123872
H89	6.5430167945	5.1359071169	9.5438759438

6^{Sc}-py-py to 9^{Sc}

Fe1	1.0121966018	0.8160023850	8.5745253702
Sc2	2.8656493870	2.5316533117	10.7375921070
Si3	2.1758576988	5.4709212490	8.8536926900
Si4	2.7863367962	-0.1944206256	12.9350588289
N5	2.3161347896	0.6923647139	11.4907115153
N6	2.1630070422	3.7480712489	9.2182836798
N7	5.0315295205	2.0683521047	10.1122015889
N8	3.6014133986	3.6838558795	12.2281638984
C9	6.6193901868	0.6893309712	8.9471557883
H10	6.8054412953	-0.0633525111	8.1884849268
C11	2.0717344814	-0.7780493683	9.4273507211

H12	3.1155926589	-1.0190886403	9.2801199935
C13	3.5354417752	4.4952917322	13.2302820622
C14	5.8684779677	4.6619860282	14.0150721529
C15	5.3271345209	1.1343378492	9.1867226847
C16	1.5631251806	0.0525409302	10.4935732581
C17	6.0285211872	2.6105505216	10.8508575478
C18	2.7353748195	-2.0616546002	12.5880759900
H19	3.4395332752	-2.3276802738	11.7915568355
H20	1.7431977937	-2.3988649434	12.2709748204
H21	3.0157431322	-2.6359773201	13.4785991679
C22	7.6537307015	1.2319964913	9.7110379764
H23	8.6804966413	0.9114477723	9.5590216991
C24	1.6394282817	0.1914847069	14.4474082040
C25	4.5707730322	0.2533988669	13.3962049186
H26	5.2468301137	0.0050516453	12.5701269374
H27	4.9023200579	-0.3143275219	14.2731040608
H28	4.6942192592	1.3171736459	13.6188000235
C29	5.7002840050	3.6797939320	11.8317470318
H30	5.4108071243	4.6275305429	11.3895648088
C31	3.6195619625	5.9743876627	7.6547341776
C32	0.1340401011	0.0991808324	10.3155941723
H33	-0.5441763343	0.6720831381	10.9332003473
C34	7.3566315963	2.1966921137	10.6663710425
H35	8.1386501383	2.6526521415	11.2616850552
C36	0.2025173188	-0.2970388079	14.1690986545
H37	-0.4532411675	-0.0713728024	15.0228670701
H38	0.1591822364	-1.3798793336	14.0040727638
H39	-0.2277441094	0.1907000543	13.2879004460
C40	4.5855709449	5.1919336370	13.9340708146
H41	4.2544618173	5.8794072846	14.7074566829
C42	6.3358699817	3.7282612890	13.0740978861
C43	3.6805905142	7.5130625715	7.5238865668
H44	4.4802301831	7.8058428540	6.8277015152
H45	3.8903086668	8.0013321982	8.4819515994
H46	2.7460047669	7.9319433028	7.1331218721
C47	1.1737379151	1.3480510435	6.5786305260
H48	1.3473215132	0.6423512320	5.7771558991
C49	3.4031072633	5.3761624932	6.2481460549
H50	4.2251073842	5.6666125701	5.5770013007
H51	2.4722746115	5.7301681846	5.7906540512
H52	3.3657116640	4.2824130649	6.2667374777
C53	2.1740692222	2.0346297454	7.3256770935
H54	3.2412812598	1.9806645443	7.1623613465
C55	0.9795122038	-1.2566272094	8.6499424179
H56	1.0461324931	-1.8928628095	7.7773652595
C57	0.5344639330	5.9960682039	8.0540552794
H58	-0.3008563181	5.8309309094	8.7438065688
H59	0.3177214754	5.4407009298	7.1363071201
H60	0.5449252632	7.0632800991	7.8037701939
C61	1.5337235407	2.8768114801	8.3094963297
C62	-0.2210095997	-0.7159920357	9.2023228411
H63	-1.2203335049	-0.8661308567	8.8161102752
C64	2.3569695953	6.4579293978	10.4599862463
H65	1.5819129625	6.1657073159	11.1769291806
H66	2.2310206584	7.5278301317	10.2568049946
H67	3.3243426405	6.3229070627	10.9515245399

C68	4.9719220664	5.4745058492	8.2024696954
H69	5.7933208557	5.7652053694	7.5307150626
H70	4.9907093605	4.3837723441	8.2959804495
H71	5.1970148449	5.9001054470	9.1884843209
C72	-0.0992844170	1.7344583345	7.0960604086
H73	-1.0583391046	1.3616490741	6.7620625068
C74	0.1183347668	2.6437257577	8.1704406563
H75	-0.6414838424	3.1007989450	8.7891489588
C76	2.1707314198	-0.5257599713	15.7087603306
H77	1.5108886031	-0.3297827195	16.5664507357
H78	3.1727552839	-0.1800941361	15.9867344492
H79	2.2158986259	-1.6135517187	15.5798747726
C80	1.5989695363	1.7081147060	14.7265437097
H81	0.9487944126	1.9221466530	15.5877880527
H82	1.2060741143	2.2654073862	13.8688509424
H83	2.5911242793	2.1118954269	14.9570594139
H84	4.4819180099	0.7347381568	8.6352780511
H85	7.0409523609	2.9559376904	13.3733444631
H86	6.4681627340	4.8785310461	14.8995009621
H87	2.5630025686	4.5901686340	13.7366484615

Coordinates for the structures optimized by ADF

6^{Sc}-py^{Ph}-iqn

Atom	X	Y	Z (Angs
1.Fe	0.514850	1.105656	8.982967
2.Sc	3.240089	2.290529	10.570896
3.Si	3.199791	5.019111	8.274584
4.Si	3.024102	-0.584702	12.711792
5.N	2.503561	0.516898	11.429923
6.N	2.768982	3.412860	8.870060
7.N	5.590199	2.491877	10.651600
8.N	3.634816	3.658431	12.171863
9.C	6.021526	1.067355	8.703767
10.C	7.811602	2.479582	9.716974
11.H	8.503268	2.078525	8.979573
12.C	1.163181	-0.754029	9.660945
13.H	1.969460	-1.344059	9.235018
14.C	2.715787	4.195603	13.039761
15.C	4.243004	3.976465	14.921072
16.C	6.478424	2.040142	9.717418
17.C	1.318686	0.201612	10.739952
18.C	6.005460	3.379597	11.586849
19.C	3.073927	-2.374079	12.048656
20.H	3.773087	-2.451109	11.200794
21.H	2.089272	-2.726933	11.709064
22.H	3.430998	-3.066360	12.828248
23.C	8.234665	3.399686	10.671711
24.H	9.265409	3.755226	10.677328
25.C	4.413479	3.763156	16.305863
26.H	3.628710	4.086069	16.992415
27.C	1.888820	-0.519608	14.289958
28.C	6.530772	1.114482	7.391884
29.H	7.219836	1.916034	7.113004

30.C	5.546285	3.114058	16.797892
31.H	5.652423	2.950269	17.870310
32.C	6.386035	2.866167	14.541465
33.H	7.159896	2.507864	13.861120
34.C	4.797142	-0.116883	13.177112
35.H	5.468378	-0.140507	12.304185
36.H	5.200112	-0.827867	13.914821
37.H	4.854312	0.886741	13.622456
38.C	5.015658	3.921869	12.580169
39.H	5.160389	5.029097	12.554171
40.C	3.602395	5.030125	6.368783
41.C	1.318604	4.363535	12.500068
42.H	0.641301	4.759989	13.264924
43.H	0.912609	3.394323	12.167509
44.H	1.307642	5.033067	11.628797
45.C	5.227072	-0.826322	6.771117
46.H	4.922487	-1.557696	6.023315
47.C	-0.003751	0.755934	10.974391
48.H	-0.243421	1.498444	11.731353
49.C	6.140270	0.185734	6.434905
50.H	6.533141	0.250385	5.422299
51.C	7.324197	3.856730	11.613760
52.H	7.602708	4.590393	12.369249
53.C	4.712254	-0.883613	8.066902
54.H	4.010710	-1.671967	8.338301
55.C	6.532418	2.654059	15.916961
56.H	7.413179	2.132545	16.296097
57.C	0.523137	-1.188326	14.018934
58.H	-0.112785	-1.123768	14.921508
59.H	0.626513	-2.254948	13.765298
60.H	-0.020492	-0.701022	13.195830
61.C	3.026961	4.502638	14.344739
62.H	2.256287	4.911390	14.999839
63.C	5.264796	3.532446	14.040286
64.C	4.210018	6.393625	5.970173
65.H	4.421513	6.404572	4.884603
66.H	5.158081	6.596611	6.491632
67.H	3.522924	7.230022	6.175071
68.C	5.099153	0.051911	9.025430
69.H	4.704051	-0.031645	10.041552
70.C	0.330587	1.391393	6.939019
71.H	0.025587	0.625391	6.229686
72.C	2.329887	4.800353	5.524042
73.H	2.586459	4.800009	4.448026
74.H	1.585031	5.595479	5.682385
75.H	1.846290	3.838379	5.749566
76.C	1.673916	1.675221	7.346045
77.H	2.574113	1.178943	6.992104
78.C	-0.215209	-0.816973	9.284649
79.H	-0.638273	-1.449468	8.508261
80.C	1.806864	6.274107	8.617993
81.H	1.602752	6.325260	9.699356
82.H	0.868838	6.009442	8.108918
83.H	2.094400	7.285998	8.290581
84.C	1.655689	2.778907	8.285991
85.C	-0.938062	0.121678	10.094785

86.H	-2.006443	0.319286	10.045209
87.C	4.725632	5.613961	9.230975
88.H	4.516052	5.627286	10.311098
89.H	4.988542	6.639325	8.930226
90.H	5.606779	4.978119	9.056125
91.C	4.628563	3.923698	6.054753
92.H	4.870936	3.915977	4.975302
93.H	4.248420	2.927814	6.322786
94.H	5.572212	4.079688	6.602083
95.C	-0.545175	2.285888	7.642689
96.H	-1.629025	2.311417	7.562063
97.C	0.257629	3.117104	8.486196
98.H	-0.101803	3.897329	9.151628
99.C	2.576329	-1.260810	15.459567
100.H	1.921063	-1.242993	16.350244
101.H	3.528843	-0.789458	15.745085
102.H	2.774913	-2.318998	15.223887
103.C	1.657768	0.947117	14.703768
104.H	1.012913	0.995356	15.600920
105.H	1.162475	1.519515	13.905732
106.H	2.598618	1.464691	14.944009

7^{Sc}-py^{Ph}-iqn

1.Fe	0.514850	1.105656	8.982967
2.Sc	3.240089	2.290529	10.570896
3.Si	3.199791	5.019111	8.274584
4.Si	3.024102	-0.584702	12.711792
5.N	2.503561	0.516898	11.429923
6.N	2.768982	3.412860	8.870060
7.N	5.590199	2.491877	10.651600
8.N	3.634816	3.658431	12.171863
9.C	6.021526	1.067355	8.703767
10.C	7.811602	2.479582	9.716974
11.H	8.503268	2.078525	8.979573
12.C	1.163181	-0.754029	9.660945
13.H	1.969460	-1.344059	9.235018
14.C	2.715787	4.195603	13.039761
15.C	4.243004	3.976465	14.921072
16.C	6.478424	2.040142	9.717418
17.C	1.318686	0.201612	10.739952
18.C	6.005460	3.379597	11.586849
19.C	3.073927	-2.374079	12.048656
20.H	3.773087	-2.451109	11.200794
21.H	2.089272	-2.726933	11.709064
22.H	3.430998	-3.066360	12.828248
23.C	8.234665	3.399686	10.671711
24.H	9.265409	3.755226	10.677328
25.C	4.413479	3.763156	16.305863
26.H	3.628710	4.086069	16.992415
27.C	1.888820	-0.519608	14.289958
28.C	6.530772	1.114482	7.391884
29.H	7.219836	1.916034	7.113004
30.C	5.546285	3.114058	16.797892
31.H	5.652423	2.950269	17.870310
32.C	6.386035	2.866167	14.541465

33.H	7.159896	2.507864	13.861120
34.C	4.797142	-0.116883	13.177112
35.H	5.468378	-0.140507	12.304185
36.H	5.200112	-0.827867	13.914821
37.H	4.854312	0.886741	13.622456
38.C	5.015658	3.921869	12.580169
39.H	5.160389	5.029097	12.554171
40.C	3.602395	5.030125	6.368783
41.C	1.318604	4.363535	12.500068
42.H	0.641301	4.759989	13.264924
43.H	0.912609	3.394323	12.167509
44.H	1.307642	5.033067	11.628797
45.C	5.227072	-0.826322	6.771117
46.H	4.922487	-1.557696	6.023315
47.C	-0.003751	0.755934	10.974391
48.H	-0.243421	1.498444	11.731353
49.C	6.140270	0.185734	6.434905
50.H	6.533141	0.250385	5.422299
51.C	7.324197	3.856730	11.613760
52.H	7.602708	4.590393	12.369249
53.C	4.712254	-0.883613	8.066902
54.H	4.010710	-1.671967	8.338301
55.C	6.532418	2.654059	15.916961
56.H	7.413179	2.132545	16.296097
57.C	0.523137	-1.188326	14.018934
58.H	-0.112785	-1.123768	14.921508
59.H	0.626513	-2.254948	13.765298
60.H	-0.020492	-0.701022	13.195830
61.C	3.026961	4.502638	14.344739
62.H	2.256287	4.911390	14.999839
63.C	5.264796	3.532446	14.040286
64.C	4.210018	6.393625	5.970173
65.H	4.421513	6.404572	4.884603
66.H	5.158081	6.596611	6.491632
67.H	3.522924	7.230022	6.175071
68.C	5.099153	0.051911	9.025430
69.H	4.704051	-0.031645	10.041552
70.C	0.330587	1.391393	6.939019
71.H	0.025587	0.625391	6.229686
72.C	2.329887	4.800353	5.524042
73.H	2.586459	4.800009	4.448026
74.H	1.585031	5.595479	5.682385
75.H	1.846290	3.838379	5.749566
76.C	1.673916	1.675221	7.346045
77.H	2.574113	1.178943	6.992104
78.C	-0.215209	-0.816973	9.284649
79.H	-0.638273	-1.449468	8.508261
80.C	1.806864	6.274107	8.617993
81.H	1.602752	6.325260	9.699356
82.H	0.868838	6.009442	8.108918
83.H	2.094400	7.285998	8.290581
84.C	1.655689	2.778907	8.285991
85.C	-0.938062	0.121678	10.094785
86.H	-2.006443	0.319286	10.045209
87.C	4.725632	5.613961	9.230975
88.H	4.516052	5.627286	10.311098

89.H	4.988542	6.639325	8.930226
90.H	5.606779	4.978119	9.056125
91.C	4.628563	3.923698	6.054753
92.H	4.870936	3.915977	4.975302
93.H	4.248420	2.927814	6.322786
94.H	5.572212	4.079688	6.602083
95.C	-0.545175	2.285888	7.642689
96.H	-1.629025	2.311417	7.562063
97.C	0.257629	3.117104	8.486196
98.H	-0.101803	3.897329	9.151628
99.C	2.576329	-1.260810	15.459567
100.H	1.921063	-1.242993	16.350244
101.H	3.528843	-0.789458	15.745085
102.H	2.774913	-2.318998	15.223887
103.C	1.657768	0.947117	14.703768
104.H	1.012913	0.995356	15.600920
105.H	1.162475	1.519515	13.905732
106.H	2.598618	1.464691	14.944009

6^{Y}-py^{Ph}-iqn

1.Fe	0.455505	1.082653	8.949800
2.Y	3.226570	2.245986	10.525573
3.Si	3.144333	5.067058	8.185289
4.Si	2.970091	-0.696185	12.730488
5.N	2.399617	0.361154	11.464519
6.N	2.683087	3.466910	8.709880
7.N	5.707693	2.516699	10.717601
8.N	3.730530	3.754836	12.218438
9.C	6.104019	1.092992	8.768985
10.C	7.918635	2.500660	9.769601
11.H	8.609850	2.104763	9.028045
12.C	1.070306	-0.802678	9.627302
13.H	1.867285	-1.410813	9.208825
14.C	2.817574	4.285053	13.089994
15.C	4.330750	4.047791	14.971622
16.C	6.591809	2.063823	9.782703
17.C	1.232399	0.111276	10.740509
18.C	6.112791	3.418846	11.644408
19.C	3.049078	-2.489581	12.095837
20.H	3.763034	-2.559694	11.259253
21.H	2.072534	-2.840284	11.730951
22.H	3.391724	-3.187475	12.876108
23.C	8.341213	3.423076	10.725339
24.H	9.372547	3.775695	10.730597
25.C	4.495284	3.839566	16.358339
26.H	3.720278	4.191580	17.039499
27.C	1.880762	-0.591049	14.328369
28.C	6.579860	1.150504	7.444727
29.H	7.269175	1.942823	7.153409
30.C	5.605303	3.159413	16.854217
31.H	5.707831	3.005310	17.929211
32.C	6.433296	2.862515	14.598763
33.H	7.196535	2.472796	13.921767
34.C	4.739764	-0.166551	13.156513
35.H	5.408677	-0.188444	12.282029

36.H	5.169135	-0.858093	13.897630
37.H	4.784674	0.842554	13.590566
38.C	5.114492	3.976217	12.634803
39.H	5.291934	5.077802	12.618136
40.C	3.609718	5.099641	6.305117
41.C	1.411336	4.428766	12.562549
42.H	0.741852	4.843239	13.323219
43.H	0.998424	3.445301	12.277045
44.H	1.376864	5.068945	11.671065
45.C	5.234786	-0.769288	6.836070
46.H	4.902647	-1.491932	6.089170
47.C	-0.072725	0.713933	10.948880
48.H	-0.301563	1.447225	11.718442
49.C	6.150553	0.230136	6.490010
50.H	6.522549	0.300479	5.467693
51.C	7.431312	3.888545	11.667445
52.H	7.718841	4.623200	12.418304
53.C	4.749571	-0.834731	8.143359
54.H	4.045910	-1.615977	8.426819
55.C	6.572829	2.654003	15.977687
56.H	7.435403	2.107810	16.359318
57.C	0.506216	-1.246442	14.072794
58.H	-0.128148	-1.166783	14.975066
59.H	0.596511	-2.316254	13.827063
60.H	-0.031761	-0.759066	13.245448
61.C	3.127219	4.598636	14.396236
62.H	2.356989	5.005053	15.052072
63.C	5.341512	3.569657	14.093891
64.C	4.233381	6.459930	5.926987
65.H	4.460591	6.486174	4.844885
66.H	5.176492	6.645098	6.465448
67.H	3.553216	7.300808	6.137401
68.C	5.180152	0.085446	9.102730
69.H	4.832040	-0.031535	10.132852
70.C	0.242583	1.352203	6.908601
71.H	-0.062701	0.571335	6.216505
72.C	2.349139	4.867023	5.444698
73.H	2.612342	4.864944	4.370684
74.H	1.599580	5.658942	5.598257
75.H	1.866534	3.904092	5.670770
76.C	1.587527	1.669384	7.282782
77.H	2.490697	1.191205	6.911121
78.C	-0.304215	-0.824847	9.231893
79.H	-0.735251	-1.439514	8.445113
80.C	1.763206	6.329782	8.538148
81.H	1.572528	6.367224	9.623035
82.H	0.819462	6.060609	8.041489
83.H	2.037630	7.347387	8.217554
84.C	1.572182	2.804682	8.185138
85.C	-1.013715	0.117202	10.050586
86.H	-2.076407	0.340273	9.994540
87.C	4.650103	5.599789	9.209271
88.H	4.413409	5.566504	10.283146
89.H	4.931184	6.634538	8.961052
90.H	5.531019	4.964940	9.031217
91.C	4.635216	3.983920	6.018799

92.H	4.906601	3.970606	4.946723
93.H	4.238724	2.992604	6.281614
94.H	5.565667	4.133349	6.590480
95.C	-0.633988	2.241993	7.618228
96.H	-1.719480	2.250568	7.558886
97.C	0.172899	3.102255	8.428097
98.H	-0.184760	3.891918	9.084007
99.C	2.578078	-1.312064	15.503074
100.H	1.933895	-1.285045	16.401268
101.H	3.531264	-0.830725	15.770915
102.H	2.782382	-2.372111	15.280571
103.C	1.669103	0.888697	14.709489
104.H	1.037792	0.965335	15.613902
105.H	1.166941	1.444518	13.904031
106.H	2.617311	1.404846	14.924829

7^{Y}-py^{Ph}-iqn

1.Fe	4.281411	9.043769	5.838856
2.Y	2.489724	6.507870	4.635008
3.Si	4.200866	6.923765	1.409984
4.Si	1.175759	5.975415	8.028274
5.N	3.970705	7.266755	3.110517
6.N	1.994264	6.933158	6.809387
7.N	0.672909	5.403907	3.453211
8.N	2.802956	4.097475	4.592682
9.C	-0.227702	6.094556	2.704475
10.C	-1.161108	5.477732	1.880957
11.H	-1.880309	6.072637	1.323442
12.C	-1.141332	4.068454	1.807749
13.H	-1.843119	3.547884	1.153159
14.C	-0.218906	3.351697	2.526544
15.H	-0.150546	2.273929	2.408802
16.C	0.727811	4.015350	3.373388
17.C	1.775358	3.319644	4.037264
18.C	1.802629	1.884463	4.318006
19.C	3.058722	1.291090	4.619668
20.C	4.279127	2.164989	4.482548
21.H	5.133611	1.754155	5.039538
22.H	4.592257	2.216832	3.416987
23.C	3.952419	3.564326	4.925592
24.C	4.990576	4.346328	5.671415
25.H	4.673027	5.366456	5.932548
26.H	5.927299	4.415934	5.095577
27.H	5.237063	3.841854	6.619977
28.C	3.144663	-0.044323	5.013017
29.H	4.127181	-0.467942	5.239666
30.C	2.003021	-0.843259	5.097605
31.H	2.082402	-1.892980	5.381374
32.C	0.753524	-0.269216	4.829622
33.H	-0.153770	-0.865685	4.927066
34.C	0.655111	1.074242	4.466636
35.H	-0.335563	1.510379	4.338849
36.C	-0.152422	7.578947	2.773791
37.C	-0.200767	8.340779	1.590292
38.H	-0.278478	7.826687	0.632420

39.C	-0.121347	9.732056	1.633958
40.H	-0.147354	10.302953	0.704609
41.C	0.005240	10.393525	2.859553
42.H	0.065626	11.482590	2.892610
43.C	0.049109	9.652059	4.040230
44.H	0.122320	10.161281	4.999336
45.C	2.961723	5.582195	0.910641
46.H	1.923380	5.927475	1.012433
47.H	3.063895	4.659463	1.501003
48.H	3.111995	5.315115	-0.146157
49.C	-0.027118	8.253661	4.000288
50.H	-0.061606	7.696353	4.942364
51.C	4.588252	8.321818	3.783390
52.C	4.147940	9.703764	3.833443
53.H	3.260863	10.083063	3.332556
54.C	5.100782	10.471679	4.576127
55.H	5.060711	11.542945	4.756668
56.C	6.117670	9.575141	5.049723
57.H	6.982863	9.849701	5.648508
58.C	5.784592	8.257092	4.602062
59.H	6.364086	7.354342	4.781057
60.C	2.826444	8.013021	7.111878
61.C	2.517310	9.418443	6.924655
62.H	1.574157	9.795513	6.543136
63.C	3.604478	10.210068	7.413592
64.H	3.648330	11.296214	7.437558
65.C	4.631725	9.314496	7.863064
66.H	5.591578	9.605200	8.283015
67.C	4.174073	7.975430	7.648823
68.H	4.716449	7.066849	7.900174
69.C	3.855572	8.471406	0.359751
70.H	2.810341	8.789863	0.501225
71.H	4.005916	8.280364	-0.714947
72.H	4.501824	9.313916	0.648405
73.C	5.981541	6.262464	1.011192
74.C	6.340836	5.127897	1.991735
75.H	7.349315	4.730022	1.775127
76.H	5.632354	4.286998	1.920596
77.H	6.333833	5.484605	3.032483
78.C	6.034173	5.705845	-0.429059
79.H	7.064252	5.389582	-0.677288
80.H	5.735512	6.458096	-1.176934
81.H	5.383089	4.826947	-0.556214
82.C	7.016355	7.399727	1.145175
83.H	8.036532	7.015577	0.959406
84.H	7.007257	7.851317	2.148879
85.H	6.831330	8.204436	0.416551
86.C	-0.164521	6.998466	8.990758
87.C	0.292636	4.566319	7.127884
88.H	0.999008	3.909064	6.600296
89.H	-0.440332	4.928500	6.391916
90.H	-0.249582	3.939207	7.851613
91.C	2.417991	5.233684	9.264880
92.H	3.116266	4.563036	8.739272
93.H	1.914460	4.639104	10.043833
94.H	3.011147	6.012661	9.767152

95.C	0.499164	8.063503	9.889487
96.H	-0.272177	8.660337	10.411012
97.H	1.125447	8.760992	9.312320
98.H	1.135512	7.605378	10.662851
99.C	-1.015986	6.059904	9.874639
100.H	-1.758816	6.646126	10.446790
101.H	-0.402923	5.509580	10.606301
102.H	-1.572229	5.320900	9.277395
103.C	-1.092454	7.696426	7.975036
104.H	-1.873517	8.278910	8.496735
105.H	-1.605649	6.971551	7.323887
106.H	-0.531162	8.390523	7.332014

6^{Lu}-py^{Ph}-iqn

1.Fe	4.273666	9.001501	5.834401
2.Lu	2.448137	6.509746	4.628552
3.Si	4.171094	6.904868	1.422102
4.Si	1.179876	5.953698	8.016787
5.N	3.920899	7.233764	3.123502
6.N	1.983269	6.905117	6.783945
7.N	0.686208	5.417468	3.452796
8.N	2.801620	4.136865	4.609646
9.C	-0.212065	6.106630	2.698040
10.C	-1.142113	5.487928	1.878901
11.H	-1.861104	6.079487	1.316486
12.C	-1.125601	4.076985	1.813457
13.H	-1.827008	3.553879	1.162487
14.C	-0.203915	3.361706	2.537925
15.H	-0.139079	2.283138	2.425530
16.C	0.741465	4.027382	3.380245
17.C	1.786872	3.344192	4.052490
18.C	1.830240	1.909887	4.335049
19.C	3.086765	1.332334	4.640293
20.C	4.298840	2.220825	4.511846
21.H	5.155385	1.821639	5.073046
22.H	4.616827	2.276620	3.448179
23.C	3.957038	3.617886	4.948542
24.C	4.980638	4.419292	5.688888
25.H	4.659558	5.448076	5.909701
26.H	5.926525	4.471732	5.125575
27.H	5.211784	3.942965	6.655846
28.C	3.188041	-0.005850	5.028134
29.H	4.172955	-0.419799	5.256743
30.C	2.053491	-0.816263	5.103712
31.H	2.143888	-1.866168	5.383675
32.C	0.799610	-0.255040	4.832645
33.H	-0.101836	-0.862829	4.924600
34.C	0.686356	1.086408	4.474794
35.H	-0.306846	1.513790	4.344804
36.C	-0.121021	7.588593	2.764096
37.C	-0.174731	8.351485	1.583216
38.H	-0.270565	7.839279	0.625346
39.C	-0.076258	9.741423	1.626520
40.H	-0.106445	10.313499	0.698371
41.C	0.075334	10.400859	2.851321

42.H	0.149549	11.488577	2.883983
43.C	0.126057	9.657233	4.030663
44.H	0.215762	10.166284	4.989166
45.C	2.943332	5.567324	0.891234
46.H	1.901713	5.903717	0.985560
47.H	3.046389	4.634077	1.464012
48.H	3.109124	5.323567	-0.168257
49.C	0.032252	8.260731	3.991731
50.H	-0.007708	7.704859	4.935573
51.C	4.557238	8.285472	3.791669
52.C	4.132431	9.671301	3.838884
53.H	3.243443	10.057200	3.345437
54.C	5.096033	10.430197	4.574492
55.H	5.063829	11.501369	4.758978
56.C	6.110131	9.525507	5.038594
57.H	6.980027	9.792858	5.633294
58.C	5.764708	8.210680	4.591381
59.H	6.339277	7.303838	4.762829
60.C	2.823187	7.979978	7.096882
61.C	2.519536	9.387052	6.925341
62.H	1.576658	9.770933	6.548897
63.C	3.612443	10.168706	7.415182
64.H	3.665123	11.254616	7.440442
65.C	4.634670	9.264017	7.858641
66.H	5.598031	9.546441	8.275854
67.C	4.167749	7.928973	7.640191
68.H	4.703228	7.016024	7.888189
69.C	3.825219	8.462957	0.396230
70.H	2.780039	8.778026	0.539811
71.H	3.979171	8.284069	-0.679844
72.H	4.470912	9.301085	0.696789
73.C	5.954085	6.254075	1.035579
74.C	6.313772	5.124224	2.020496
75.H	7.326377	4.733300	1.811534
76.H	5.611250	4.278620	1.943236
77.H	6.296137	5.480439	3.060826
78.C	6.017288	5.690323	-0.401937
79.H	7.051144	5.379666	-0.641983
80.H	5.717864	6.436162	-1.157008
81.H	5.373041	4.805530	-0.526952
82.C	6.981875	7.397642	1.169413
83.H	8.002867	7.020745	0.974417
84.H	6.976267	7.844506	2.175164
85.H	6.787206	8.204489	0.445358
86.C	-0.145558	6.986095	8.978559
87.C	0.281710	4.540498	7.141060
88.H	0.977304	3.872361	6.613359
89.H	-0.460122	4.897923	6.412070
90.H	-0.253810	3.926551	7.880218
91.C	2.444422	5.223525	9.232695
92.H	3.144709	4.565423	8.694993
93.H	1.956586	4.618075	10.012841
94.H	3.032829	6.006999	9.732334
95.C	0.526864	8.051616	9.869555
96.H	-0.239935	8.656000	10.388707
97.H	1.156876	8.741760	9.287716

98.H	1.161149	7.593277	10.644616
99.C	-0.999598	6.055949	9.868647
100.H	-1.736569	6.648928	10.441508
101.H	-0.386372	5.504382	10.600092
102.H	-1.562688	5.318262	9.275744
103.C	-1.070945	7.682436	7.960243
104.H	-1.853411	8.264126	8.480007
105.H	-1.581698	6.956499	7.308641
106.H	-0.509250	8.376827	7.318095

7^{Lu}-py^{Ph}-iqn

1.Fe	0.477135	1.091845	8.963103
2.Lu	3.253374	2.246281	10.518677
3.Si	3.121351	5.066004	8.176578
4.Si	2.955376	-0.699831	12.722941
5.N	2.430950	0.376326	11.448772
6.N	2.697704	3.460894	8.726697
7.N	5.699400	2.521502	10.715766
8.N	3.727904	3.702792	12.224568
9.C	6.093611	1.102830	8.774745
10.C	7.915843	2.500843	9.780082
11.H	8.608821	2.103208	9.040719
12.C	1.073999	-0.801522	9.633628
13.H	1.862616	-1.418222	9.212020
14.C	2.812806	4.258185	13.083531
15.C	4.328188	4.046728	14.970547
16.C	6.587853	2.068905	9.784730
17.C	1.250268	0.122311	10.735572
18.C	6.108334	3.409246	11.653316
19.C	3.000838	-2.489779	12.081709
20.H	3.728034	-2.584436	11.259943
21.H	2.021608	-2.816070	11.702309
22.H	3.308611	-3.192142	12.872694
23.C	8.338049	3.417379	10.742059
24.H	9.369983	3.768359	10.753392
25.C	4.496725	3.858785	16.359674
26.H	3.723881	4.221852	17.040031
27.C	1.858003	-0.599382	14.313037
28.C	6.562234	1.155093	7.448598
29.H	7.255137	1.942927	7.152546
30.C	5.609898	3.187352	16.860865
31.H	5.717735	3.047294	17.937661
32.C	6.435599	2.863448	14.608540
33.H	7.199504	2.470285	13.934649
34.C	4.728169	-0.207876	13.170308
35.H	5.405208	-0.254689	12.303439
36.H	5.131787	-0.901995	13.922100
37.H	4.788378	0.804071	13.594755
38.C	5.105694	3.955778	12.638275
39.H	5.261250	5.061174	12.614080
40.C	3.587738	5.097672	6.296823
41.C	1.417199	4.413551	12.537427
42.H	0.736503	4.833042	13.286766
43.H	1.003985	3.434227	12.238920
44.H	1.405066	5.057193	11.646197

45.C	5.200769	-0.759289	6.858119
46.H	4.860715	-1.484039	6.117048
47.C	-0.050469	0.727740	10.958795
48.H	-0.270075	1.460574	11.731291
49.C	6.119492	0.233684	6.500923
50.H	6.484422	0.297879	5.475365
51.C	7.425991	3.877890	11.684362
52.H	7.710822	4.606312	12.443023
53.C	4.723155	-0.817735	8.168574
54.H	4.018348	-1.595252	8.460947
55.C	6.576623	2.670416	15.988518
56.H	7.439571	2.129181	16.377203
57.C	0.484175	-1.260407	14.067559
58.H	-0.147192	-1.168078	14.970754
59.H	0.577313	-2.334133	13.840373
60.H	-0.058794	-0.789029	13.234196
61.C	3.121957	4.584782	14.384934
62.H	2.356189	5.013164	15.031599
63.C	5.339900	3.562981	14.098537
64.C	4.215149	6.459545	5.925389
65.H	4.449902	6.485465	4.844696
66.H	5.155395	6.644138	6.469962
67.H	3.533924	7.301635	6.130707
68.C	5.164989	0.104030	9.121397
69.H	4.826927	-0.008551	10.155659
70.C	0.245928	1.352516	6.921836
71.H	-0.063665	0.569214	6.234032
72.C	2.331655	4.872310	5.427056
73.H	2.605657	4.871338	4.355585
74.H	1.585670	5.669130	5.573455
75.H	1.842334	3.911099	5.645457
76.C	1.593313	1.672103	7.285297
77.H	2.494659	1.197430	6.904765
78.C	-0.302121	-0.809374	9.242799
79.H	-0.740710	-1.414629	8.452824
80.C	1.719304	6.304849	8.501858
81.H	1.517048	6.370146	9.582627
82.H	0.784767	6.013073	8.001286
83.H	1.986768	7.315859	8.155075
84.C	1.580722	2.797676	8.198174
85.C	-0.999923	0.140013	10.062992
86.H	-2.059669	0.376400	10.005300
87.C	4.612452	5.632880	9.199832
88.H	4.379838	5.586078	10.273591
89.H	4.865377	6.675703	8.959287
90.H	5.508489	5.022350	9.013741
91.C	4.614455	3.986387	6.001006
92.H	4.885993	3.988746	4.928911
93.H	4.219317	2.990514	6.248112
94.H	5.543754	4.129814	6.575850
95.C	-0.627008	2.240440	7.637298
96.H	-1.713172	2.244083	7.587848
97.C	0.183646	3.102074	8.442133
98.H	-0.171346	3.891315	9.100128
99.C	2.558403	-1.321229	15.485960
100.H	1.914350	-1.294372	16.384311

101.H	3.512422	-0.841431	15.753662
102.H	2.760748	-2.381804	15.262389
103.C	1.646864	0.878813	14.696454
104.H	1.027707	0.953409	15.609084
105.H	1.131937	1.432363	13.897727
106.H	2.596763	1.396741	14.898576

6^{Sc}-qn-iqn

1.Fe	9.065073	3.696267	10.606605
2.Sc	6.953584	3.943139	8.029656
3.Si	4.285023	3.191581	10.257824
4.Si	9.392229	5.879820	6.323795
5.N	5.986358	3.308198	9.771845
6.N	8.820003	4.789615	7.600402
7.N	5.595121	5.622490	7.392183
8.N	5.844114	3.156750	6.213163
9.C	4.920970	4.059015	5.709752
10.C	4.854513	5.377584	6.228824
11.C	5.911911	1.880703	5.673367
12.C	3.968469	3.616131	4.726021
13.H	3.164664	4.290760	4.446251
14.C	6.887933	0.959275	6.151109
15.C	5.404082	6.690526	8.126329
16.C	6.975188	-0.312590	5.591389
17.H	7.737665	-0.997710	5.968287
18.C	6.268621	6.986203	9.310506
19.H	7.077389	6.257021	9.446148
20.H	5.668224	7.012369	10.234570
21.H	6.729730	7.981642	9.203778
22.C	5.031572	1.442836	4.634213
23.C	6.112291	-0.733815	4.565872
24.H	6.201228	-1.737475	4.151126
25.C	3.926392	7.666365	6.382260
26.C	7.810954	1.375430	7.257029
27.H	8.515803	0.581453	7.531126
28.H	7.239972	1.589053	8.183580
29.H	8.422752	2.253147	6.971752
30.C	3.947803	6.624551	4.201433
31.H	4.243561	5.812674	3.539663
32.C	4.197463	6.521662	5.592734
33.C	5.144738	0.142682	4.099426
34.H	4.452264	-0.160906	3.311815
35.C	4.020539	2.359825	4.207460
36.H	3.274695	2.029259	3.482088
37.C	3.079642	8.874370	4.449041
38.H	2.637115	9.772319	4.017149
39.C	3.385341	8.820874	5.810406
40.H	3.193324	9.687007	6.448220
41.C	3.377080	7.767120	3.646171
42.H	3.188034	7.802811	2.572324
43.C	4.239377	7.603130	7.856939
44.H	4.434629	8.608121	8.262870
45.H	3.367227	7.211002	8.423758
46.C	6.990799	3.178358	10.744966
47.C	11.107109	3.557151	10.244398

48.H	11.776291	2.840763	10.714309
49.C	8.403637	3.578126	12.575070
50.H	8.882192	4.058291	13.424910
51.C	10.386682	3.364561	9.024029
52.H	10.436053	2.485965	8.386543
53.C	9.622557	4.565503	8.729747
54.C	7.379589	4.146465	11.753149
55.H	6.933801	5.129888	11.874684
56.C	3.893056	1.578867	11.268113
57.C	8.699844	2.266947	12.073177
58.H	9.441796	1.581918	12.475567
59.C	8.126815	5.828036	4.921547
60.H	7.982092	4.807535	4.535959
61.H	8.461513	6.460036	4.084977
62.H	7.145964	6.207703	5.241289
63.C	7.855083	2.026936	10.945104
64.H	7.823415	1.112695	10.358288
65.C	12.255600	5.560166	6.639734
66.H	13.225929	5.265985	6.198841
67.H	12.106032	4.954704	7.546068
68.H	12.344414	6.612779	6.950213
69.C	9.859387	5.469285	9.839911
70.H	9.428248	6.462083	9.936771
71.C	3.785962	4.704090	11.309900
72.H	4.412066	4.815556	12.207500
73.H	2.737634	4.626543	11.640538
74.H	3.872645	5.627552	10.716431
75.C	4.414863	0.347983	10.497828
76.H	4.177907	-0.580638	11.048529
77.H	5.505628	0.387386	10.364954
78.H	3.958131	0.265256	9.499570
79.C	11.124967	5.360349	5.607203
80.C	3.228854	3.202426	8.690382
81.H	3.456921	2.350299	8.032371
82.H	3.374845	4.121957	8.104514
83.H	2.161249	3.148805	8.953227
84.C	4.533256	1.618793	12.672924
85.H	4.288849	0.693509	13.226486
86.H	4.156708	2.464358	13.269729
87.H	5.629544	1.699470	12.630895
88.C	2.362161	1.444867	11.437904
89.H	2.129281	0.540267	12.028985
90.H	1.841946	1.349808	10.472883
91.H	1.927517	2.303140	11.975019
92.C	10.781700	4.860523	10.748740
93.H	11.160137	5.300935	11.667777
94.C	9.508614	7.660014	6.995168
95.H	10.191938	7.732713	7.854309
96.H	8.515220	8.008440	7.317583
97.H	9.867196	8.358626	6.222325
98.C	11.445268	6.226529	4.367599
99.H	12.434318	5.946864	3.960609
100.H	11.487757	7.299736	4.613028
101.H	10.708996	6.092649	3.561167
102.C	11.077879	3.878596	5.178587
103.H	12.049174	3.569416	4.750730

104.H	10.308766	3.697568	4.411993
105.H	10.865153	3.217715	6.031417

7^{Sc}-qn-iqn

1.Fe	9.064294	3.695723	10.606182
2.Sc	6.953928	3.943072	8.029542
3.Si	4.284354	3.193506	10.256911
4.Si	9.390573	5.881737	6.324198
5.N	5.986102	3.309550	9.771198
6.N	8.819535	4.790634	7.601105
7.N	5.596137	5.621522	7.392436
8.N	5.844856	3.155660	6.213256
9.C	4.921695	4.058082	5.710100
10.C	4.855745	5.376812	6.228982
11.C	5.912429	1.879741	5.673468
12.C	3.969191	3.615421	4.726308
13.H	3.165104	4.289783	4.446959
14.C	6.888409	0.958147	6.151055
15.C	5.406582	6.690040	8.126373
16.C	6.975485	-0.313608	5.591095
17.H	7.737940	-0.998691	5.967885
18.C	6.270667	6.984134	9.311253
19.H	7.079611	6.254951	9.445923
20.H	5.669980	7.008527	10.235189
21.H	6.731221	7.980089	9.206456
22.C	5.031929	1.441902	4.634367
23.C	6.112469	-0.734612	4.565508
24.H	6.201122	-1.738141	4.150625
25.C	3.927740	7.665740	6.382766
26.C	7.812078	1.374413	7.256453
27.H	8.515345	0.579802	7.532484
28.H	7.241037	1.590155	8.182566
29.H	8.424965	2.250787	6.969758
30.C	3.946784	6.623410	4.202280
31.H	4.241746	5.811584	3.540204
32.C	4.197987	6.520753	5.593411
33.C	5.144783	0.141823	4.099415
34.H	4.452156	-0.161643	3.312011
35.C	4.021130	2.359147	4.207652
36.H	3.275347	2.028735	3.482234
37.C	3.079464	8.873615	4.449884
38.H	2.637133	9.771752	4.018138
39.C	3.385699	8.819913	5.811132
40.H	3.194855	9.686177	6.449223
41.C	3.376149	7.766048	3.647136
42.H	3.186045	7.801281	2.573412
43.C	4.243324	7.604492	7.856937
44.H	4.441848	8.609926	8.260385
45.H	3.371427	7.215922	8.426708
46.C	6.990424	3.178204	10.744117
47.C	11.106619	3.556903	10.244567
48.H	11.775880	2.840185	10.713893
49.C	8.402998	3.576258	12.574842
50.H	8.881531	4.055695	13.425121
51.C	10.386470	3.364878	9.023943
52.H	10.436038	2.486558	8.386140

53.C	9.622249	4.565941	8.730177
54.C	7.379314	4.145420	11.753198
55.H	6.933695	5.128877	11.875246
56.C	3.893753	1.580744	11.268083
57.C	8.699068	2.265393	12.071898
58.H	9.441110	1.580251	12.473801
59.C	8.125476	5.829128	4.921819
60.H	7.981692	4.808008	4.537442
61.H	8.460403	6.460149	4.084708
62.H	7.144200	6.208566	5.240378
63.C	7.854343	2.026303	10.943577
64.H	7.822545	1.112419	10.356260
65.C	12.254266	5.560018	6.639990
66.H	13.224459	5.265786	6.198979
67.H	12.104301	4.953908	7.545863
68.H	12.343300	6.612299	6.950999
69.C	9.858973	5.469292	9.840724
70.H	9.428030	6.462157	9.937617
71.C	3.785002	4.706108	11.308682
72.H	4.410513	4.816773	12.206784
73.H	2.736554	4.627911	11.638716
74.H	3.872080	5.630001	10.716251
75.C	4.415957	0.349982	10.497912
76.H	4.180795	-0.578379	11.049844
77.H	5.506630	0.390420	10.363731
78.H	3.958162	0.266357	9.500165
79.C	11.123682	5.361121	5.607235
80.C	3.228811	3.203117	8.689120
81.H	3.458825	2.351195	8.031518
82.H	3.373777	4.122642	8.103127
83.H	2.161064	3.147763	8.951028
84.C	4.534310	1.621068	12.672748
85.H	4.290408	0.695642	13.226265
86.H	4.157689	2.466498	13.269477
87.H	5.630662	1.702078	12.630730
88.C	2.363039	1.445554	11.438536
89.H	2.131145	0.540550	12.029356
90.H	1.842114	1.350681	10.473957
91.H	1.928356	2.303197	11.976543
92.C	10.780963	4.859972	10.749496
93.H	11.159052	5.299851	11.668917
94.C	9.507880	7.661796	6.995471
95.H	10.191940	7.733838	7.853993
96.H	8.515017	8.011496	7.318515
97.H	9.866730	8.359690	6.222150
98.C	11.445302	6.227077	4.367852
99.H	12.434199	5.946350	3.960989
100.H	11.489006	7.300184	4.613478
101.H	10.709376	6.094283	3.561021
102.C	11.075741	3.879328	5.178788
103.H	12.047246	3.568925	4.751917
104.H	10.307222	3.698636	4.411422
105.H	10.861699	3.218980	6.031708

References:

(1) Carver, C. T.; Monreal, M. J.; Diaconescu, P. L. *Organometallics* 2008, *27*, 363-370.
(2) Rubottom, G. M.; Evain, E. J. *Tetrahedron* 1990, *46*, 5055-5064.